Enhancing Environment, National Security, and Health

Earth and Environmental Sciences 1997 Annual Report

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Front cover (bottom):

The Center for Accelerator Mass Spectrometry's nuclear microprobe facility provides new capabilities for quantitative elemental and density microanalysis of biological, materials science, and particulate specimens.

Back cover (from left to right):

Tiltmeters are used in oil fields to monitor deep rock cracking, helping drillers locate the best places to sink additional wells. This new tiltmeter increases monitoring depth from 6000 feet to more than 10,000 feet.

The Program for Climate Model Diagnosis and Intercomparison works to improve global climate projections by developing computer simulations that can reproduce observed temperature records (example shows modeled near-surface temperature changes from 1979 to 1993).

The Geographic Information Sciences Center offers databases of environmental, demographic, infrastructure, and other spatially referenced (location-specific) data.

Cleanup technologies developed at Livermore—hydrous pyrolysis/oxidation and dynamic underground stripping—are being used to remediate soil and groundwater contamination 5000 times faster than the standard pump-and-treat process.

The National Atmospheric Release Advisory Center monitors and predicts the dispersion of hazardous materials released into the atmosphere (example shows surface concentrations simulated for a release from the Diablo Canyon nuclear power plant in California).

Contents

Dedicated to the memory of

Dr. Caroline Holloway

Director of the Center for Accelerator Mass Spectrometry
from April 1997 to February 1998

Enhancing Environment, National Security, and Health

Engagement and Accomplishment

J. C. Davis

The central theme of the Earth and Environmental Sciences (E&ES) Directorate is the application of its skills in earth and environmental sciences and technologies to a broad range of the Laboratory's missions. A good measure of success for a multi-sponsor, multi-disciplinary organization such as ours is the extent to which we engage issues of national importance and the significance of our accomplishments with respect to those issues. Another measure, posed by Director Tarter, is whether we are sought after as "solvers of problems."

Against these measures, we find that 1997 was a year of considerable success. The Directorate is engaged across the range of Laboratory and Department of Energy (DOE) missions, and is strongly coupled to the University of California (UC) and other agencies, with involvement in international issues and research as well. In several mission areas we have demonstrated excellence in modeling and simulation and in measurement and interpretation, coupling these activities to yield impressive "experiments of scale" in environmental cleanup and new insights into the global climate system.

Events both external and internal to the Laboratory have influenced our programs. The Comprehensive Test Ban Treaty has been submitted to the Senate and the Kyoto Agreement will follow. We will have a major role to play in providing the science underlying ratification of these accords. The major projects of the Stockpile Stewardship Program touched us during the year. As excavation of the National Ignition Facility (NIF) began, we used the opportunity to study the subsurface of our own site to a level of detail not previously possible, improving our plans for accelerated site cleanup. When the El Niño rains arrived, we returned the favor to NIF, providing meteorological advice that helped minimize construction delays. The accelerating pace and growing reality of the Accelerated Strategic Computing Initiative (ASCI) has led us to focus on advanced simulation as a theme of excellence for the Directorate. We now have projects in place to apply this powerful tool to global climate change and atmospheric dispersion of hazardous materials, to the safe and secure disposition of nuclear waste, and to the seismic issues of both the test ban treaty and earthquake hazards. Having committed to simulation as a tool, we are also strong proponents of the need to develop data sets and records to test such simulations—and are doing so for all of the topics above.

This document, like our first report last year, is intended to be a representative, not exhaustive, presentation of significant Directorate accomplishments. Still, the list of representative significant accomplishments is impressive. We designed the emplacement conditions for the safely

executed HOLOG sub-critical plutonium experiment at the Nevada Test Site, and had an enormous technical and economic success with the test of cleanup technologies at the poleyard facility in Visalia, California—both examples of the “experiments of scale” to which we aspire. Within the Laboratory, we have successfully brought into operation the Molten Salt Demonstration facility and a new accelerator-based ion microprobe shared with Sandia National Laboratories. A major modeling and simulation project has begun in support of the Yucca Mountain Project and we are playing a key role in the discussions between DOE’s Energy Research and Defense Programs to create an initiative to accelerate climate prediction.

Our growing relationships with other agencies suggest that we are now recognized as important elements in the solutions to their problems. We supported the U.S. Geological Survey in a very successful investigation of the seismic history of the Hayward Fault. The Survey has begun a new program in paleoseismicity of the Bay Area, in which we are a partner. We remain involved with both the Department of the Interior and the State of California in discussions of measurements that will resolve the fate of the proposed Ward Valley Disposal Site. We continue to support the Orange County Water District in their analysis of the complex groundwater system they must manage. With the National Center for Atmospheric Research, the National Aeronautics and Space Administration, and Los Alamos National Laboratory, we are discussing creation of the next-generation Community Climate Model, designed to run on ASCI-class machines. With UC, we have helped design a state-wide conference on anticipatory research. All of these interactions and relationships are strategic, not random, and align with the creation of the E&ES strategic plans.

In support of our strategy, we have led in establishing a four-Directorate Hazards Mitigation Center, have created a Geographic Information Sciences Center to support several program areas, and are proposing a Center for Fuels Assessment to resolve complex energy–environmental problems in transportation systems. Our partnership with the Nonproliferation, Arms Control, and International Security Directorate in modeling the fate and transport of chemical and biological agents for both anticipatory and response purposes continues to grow in size and importance to both them and us.

The quality and breadth of the Directorate’s work and the importance of the missions and agencies with which it is engaged are such that questions of single focus are no longer troubling. We are doing exceedingly well in multiple areas; we would not do better by limiting ourselves. We are resource-limited, not creativity-limited. The program is excellent, becoming better recognized nationally, and poised for growth.

In Situ Destruction of Contaminants by Hydrous Pyrolysis/Oxidation

Robin Newmark, Roger Aines, Kevin Knauss, Roald Leif, Marina Chiarappa, Bryant Hudson, Charles Carrigan, Andy Tompson, and Jim Richards

Lawrence Livermore has an ongoing research effort in *in situ* thermal degradation of underground contaminants such as petroleum distillates and chlorinated hydrocarbons. Our experimental work suggests that *in situ* hydrous pyrolysis/oxidation (HPO) may form the basis for a whole new approach to remediation. Far faster than other techniques, the technology provides a relatively inexpensive way to clean up difficult kinds of contaminants that plague dozens of waste sites across the country.

In 1997, we conducted a field test of HPO at a commercial application of Dynamic Underground Stripping, previously developed by Livermore and the University of California–Berkeley. The site, the Visalia Pole Yard in southern California, is designated one of the country's worst hazardous waste sites under the national Superfund program. Collaborating with and leveraging efforts funded by the Department of Energy, Livermore Laboratory Directed Research and Development, and Southern California Edison Co., the site owner, the project team brought together Livermore's expertise in geochemistry, underground imaging, noble-gas-tracer monitoring, flow and transport, supercomputer modeling, and accelerator mass spectrometry. The results of these field experiments constrain the destruction rates throughout the site, and enable Edison to make accurate estimates of total *in situ* destruction based on the recovered carbon. For their efforts, the team was recognized with the Laboratory Director's Performance Award.

Field Tests with Visalia Pole-Tar Contaminants

At Visalia, the Southern California Edison Co. and SteamTech Environmental Services are applying the Dynamic Underground Stripping thermal remediation method to clean up a large site (more than 4 acres) contaminated with pole-treating compounds (primarily creosote and pentachlorophenol) and an oil-based carrier fluid. This is a full-scale cleanup to a depth of about 100 feet, during which initial mobilization and extraction of contaminants is enhanced by combined steam/air injection in order to increase destruction of residual contaminants by HPO. Edison estimates that as much as 20 railroad tank-cars of creosote (40,000–80,000 gallons) may be present in the soil. The soil conditions are very similar to those at Livermore, the site initially proposed for a field test of HPO.

Laboratory tests at Livermore (Figure 1) indicated that the Visalia contaminants would oxidize at HPO destruction rates similar to those measured for trichloroethylene, the focus of our previous work. Dissolved oxygen reacted extensively with the compounds present in pole tar to form oxygenated products ranging from intermediates, like phenols and carboxylic acids, to the ultimate product, carbon dioxide. None of the initially detected hydrocarbons or chlorinated hydrocarbons remained following the hydrothermal treatment when sufficient oxygen was present to oxidize them all. Concentrations of all the contaminants were lowered by the hydrous pyrolysis reaction. The only new products formed, other than carbon dioxide, were oxygenated phenols and carboxylic acids, which are innocuous compounds.

Field Methods

In order to evaluate the progress of the chemical destruction *in situ*, we developed field methods for sampling and analyzing hot water for contaminants, intermediates, and products of reaction. Since HPO is an aqueous-phase reaction, it is essential to capture the fluid chemistry for evaluation. At elevated temperatures, many of the key constituents are sufficiently volatile that traditional sampling techniques are not suitable. We developed new

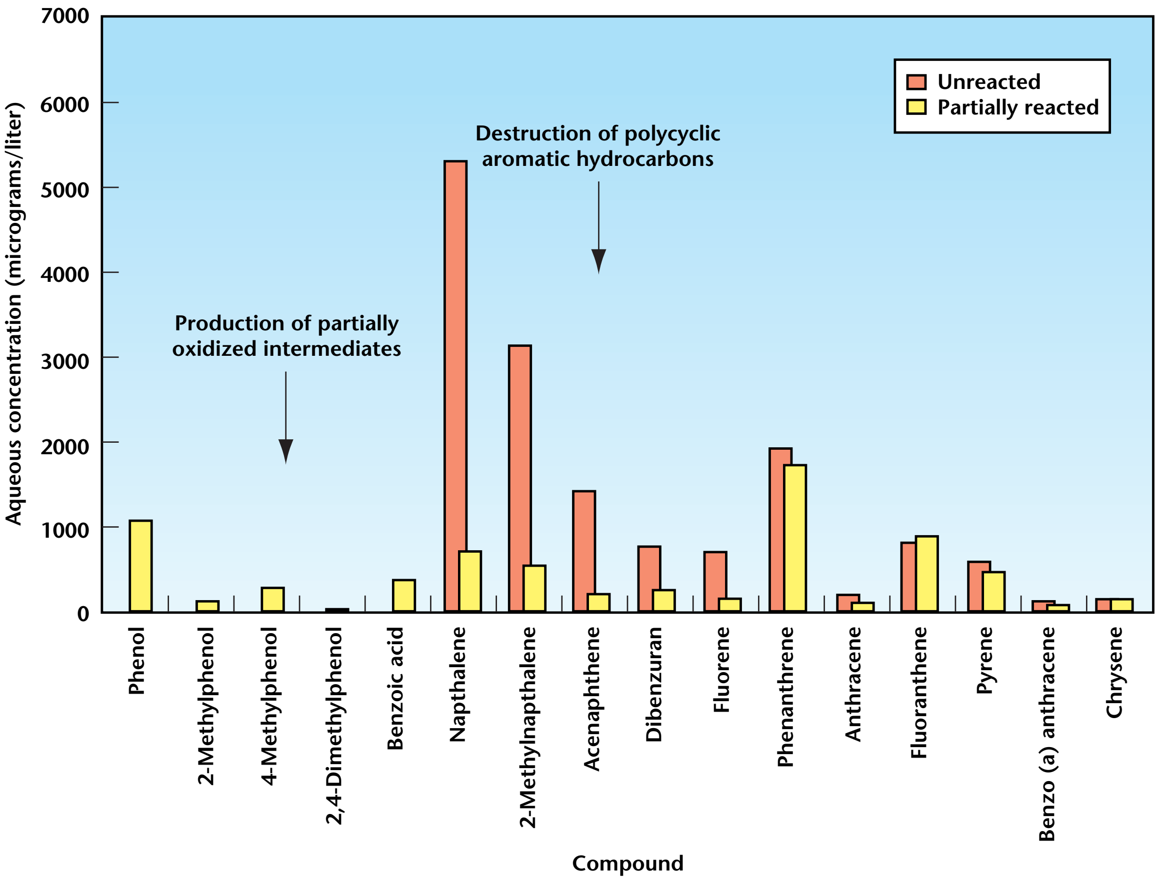

Figure 1. **In a laboratory test of the efficacy of the HPO process on the Visalia contaminants, groundwater contaminated with pole-tar compounds was initially heated in the presence of insufficient oxygen for complete oxidation (partially reacted); then the experiment was allowed to continue with sufficient oxygen to fully oxidize all the compounds. None of the hydrocarbons or chlorinated hydrocarbons initially detected in the contaminated groundwater remained following the HPO treatment (complete destruction of creosote was achieved at 120°C).**

high-temperature packer and pump systems capable of delivering a pressurized isolated fluid stream to the surface, where in-line analysis can be performed. At Visalia, an additional challenge was the protection of existing plastic monitoring wells from temperature-induced collapse. We modified the packer systems to provide circulating cooling fluids both to protect these wells and to permit their sampling during steam injection. These systems have performed successfully during the first several months of steam operations.

Since the addition of air or oxygen to the contaminated region is a critical aspect of HPO, we used noble-gas tracers to track the movement of the steam (and subsequent condensation to liquid water) and other gases initially present in the steam. This was particularly important since the HPO testing was being conducted in parallel with a full-field steam mobilization. The tracers permit us to follow the injected steam/water/oxygen pattern from a single injection well, measuring how well mixing occurs, how oxygen is consumed and

carbon dioxide produced/transported, how the intermediate HPO destruction products correlate with temperature and oxygen, and identifying the isotopic content of the extracted carbon forms. The combination of accurate fluid sampling and tracking of the injected fluids allow us to reliably diagnose the amount of *in situ* destruction occurring in the treated region.

Modeling

The subsurface conditions are complex, involving multiple phases and phase changes combined with mass and heat transport. We used advanced numerical modeling to interpret the results of the experiments. These calculations, based on a three-dimensional groundwater-modeling code developed at LLNL (NUFT). It includes individual gas properties in the multi-phase system, give tracer concentrations in time and space that are directly comparable to measurements. The modeling predicted steam and tracer movement to within an hour or two in most instances. Modeling also effectively predicted the time of "thermal breakthrough," which occurs when sufficient heat has built up in the subsurface for vaporization of contaminants to begin, and "steam collapse," which is the opposite phenomenon.

Results

Strong dispersive mixing of oxygen, contaminant, and hot water is a critical aspect in promoting HPO. The first field test focused on this hydrology aspect. Large mixing of the tracers was observed, which is in good agreement with calculations using realistic random-permeability field realizations in the subsurface model. We found that the ratio of tracer gas to natural air mixed into water was much greater than predicted by the model's initial assumption of no mixing of the injected steam and native groundwater. The increase shows that the process is more efficient than envisioned and favors the success of HPO in the field.

Evidence of the progress of HPO can be seen in the disappearance of dissolved oxygen (consumed through the HPO reactions), the appearance of oxidized intermediates, the production of carbon dioxide (a final product of HPO), and the provenance of the carbon it contains (indicating the destruction of contaminant rather than other carbon sources). In our second experiment, which involved supplementing the steam with air injection to increase the dissolved oxygen available for HPO, positive evidence of HPO was found on all counts. (A surprising finding was evidence of HPO occurring during and after the first experiment, which did not include the supplemental air.)

Dissolved oxygen decreased in fluids during both tests, from initial readings of more than 4 parts per million (ppm) to nearly 1 ppm after the second steam collapse (Figure 2).

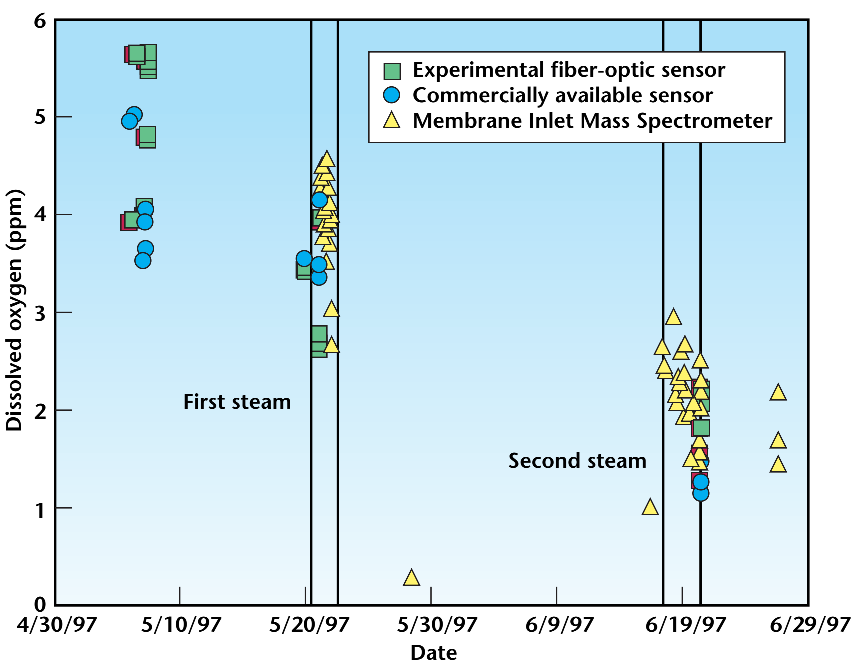

Figure 2. The disappearance of dissolved oxygen (measured in groundwater using three different methods) indicates that it is being consumed through the HPO reactions.

The decreases occurred most prominently immediately after steam collapse, indicating the consumption of oxygen during HPO. Our measurements of oxidized intermediates in the Edison extraction wells increased dramatically after Edison shut off the steam in mid-July. Simple oxidates (benzoic acid, phenol, methyl phenols) measured during the field tests make up almost 1% of the extracted organics sampled after collapse. These intermediates have a short lifetime, so a 1% concentration represents a large, but as yet unquantified, destruction rate.

Carbon dioxide, the final product of the HPO reaction, was measured in the vapor phase present both in the injection well and in the primary extraction well used for Livermore's testing. This steam-rich vapor consists of a steam–carbon-dioxide mixture with small amounts of air. The water in the extraction well also contained large amounts of oxidized intermediate products. Carbon isotopic analyses were conducted to confirm the origin of the carbon present in the carbon dioxide gas.

Our results from vapor extracted from individual wells used in our tests indicate that a sizable fraction (30–40%) of the carbon dioxide recovered from the reaction zone is derived from the contaminant (Figure 3). Dissolved bicarbonate in the water diverges much less from baseline values, indicating that most of the carbon dioxide being generated by HPO either does not equilibrate with groundwater or, more likely, is being generated principally in the unsaturated zone. Calculations of carbon balance for the entire site as of October 14, 1997, indicated that 23,000–28,000 kilograms of contaminants were destroyed.

Site Cleanup

Edison achieved full initial heating of the Visalia site by the end of July 1997 (more than 500,000 cubic yards at 100°C or above). Between late June and early August, approximately 300,000 pounds of contaminant was either removed or destroyed (an amount that would have required 600 years for removal by the previous method, pump-and-treat, which removed about 10 pounds per week). About 20,000 gallons of liquid contaminant was removed during this period, which is currently stored in temporary tanks on site.

After the initial heating phase, Edison adopted a huff-and-puff mode of operation, where steam is injected for about a week, and

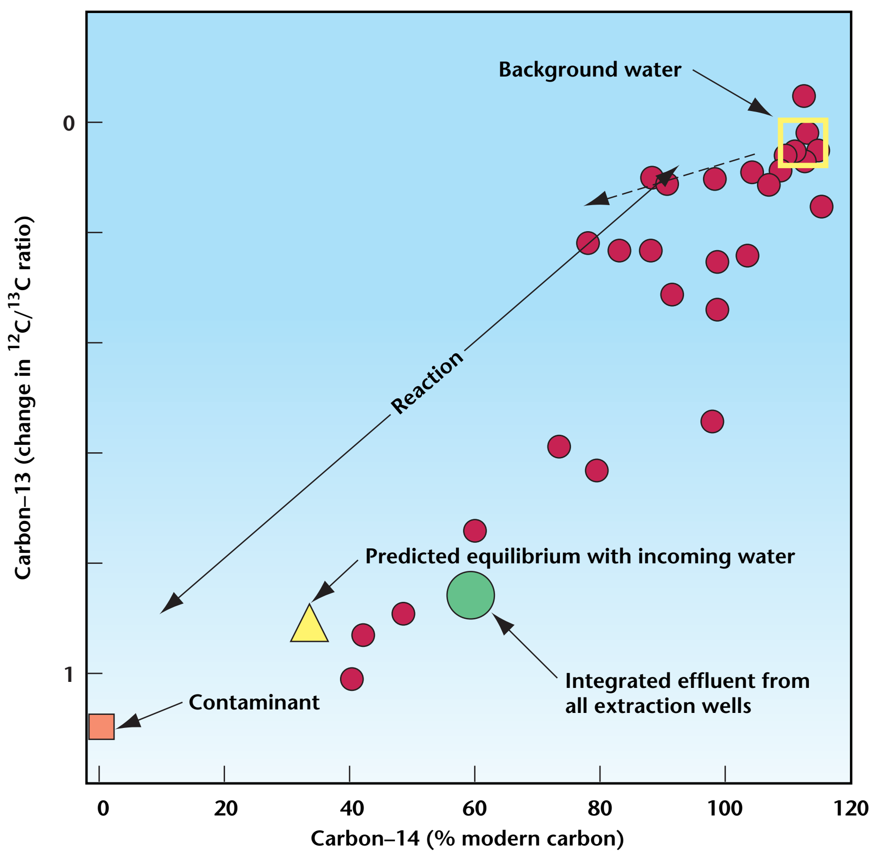

Figure 3. The carbon isotopic signatures of Visalia water and vapor samples measured after steam injection began (circles) fall between those of the background water and of the contaminant, indicating that they contain carbon released by HPO destruction of the contaminant. The integrated effluent measured on 12/16/97 falls close to the value predicted assuming equilibrium with groundwater entering the treated area (the amount of carbon entering the system equals the amount leaving if all the carbon dioxide in the system is produced by oxidation of contaminant).

then injection ceases for several days to a week while extraction continues. Maximum contaminant removal is obtained during this steam-off period as the formation fluids flash to steam under an applied vacuum. In the late fall of 1997, Edison began injecting air along with steam to enhance HPO destruction. In addition, steam and air injection commenced in the central part of the field to clean the remaining cool spots. Air injection increased HPO to 800 pounds per day from an average of 300 pounds per day obtained in the early fall. Contaminant concentrations in five of the seven extraction wells are decreasing. The cleaning process appears to be moving from the periphery inward, as expected. During nine months of operation, 565,000 pounds of creosote compounds have been removed, of which about 15% was destroyed *in situ* by HPO. Continued destruction by HPO is indicated by the high levels of carbon dioxide removed through vapor extraction.

Future Work

Work at Visalia is not yet complete. The best estimates today are that cleanup will be completed in a year, with another four years of monitoring the site. Southern California Edison had expected to meet Environmental Protection Agency requirements in about 120 years using traditional pump-and-treat technology combined with enhanced bioremediation. Instead, a piece of real estate that had been a major liability will soon become a valuable asset.

Simulating the Lifetime of a Nuclear Waste Repository Using Livermore's New Computational Capabilities

William Glassley, John Nitao, Thomas Buscheck, James Johnson, Jesse Yow, and Kenneth Jackson

Responsible management of nuclear materials ultimately requires the ability to safely and securely dispose of high-level nuclear waste. A significant inventory of this material currently exists from the U.S. defense complex and nuclear power industry, maintained at a variety of locations across the country. Successful disposition of these nuclear materials is essential for the long-term success of most major Department of Energy and U.S. nuclear programs and for the U.S. nuclear power industry. Yucca Mountain, Nevada, is currently the only candidate site for a geologic repository to receive this high-level waste and spent fuel.

Yucca Mountain (Figure 1) is seen as a potentially suitable repository site because of its arid climate, remote location, geologic setting, and the geochemical and hydrologic properties of the host rock materials. Particularly important is the characteristic of the site that the ambient water table is hundreds of feet below the potential repository location. The absence of any significant volume of liquid water passing through the potential repository dramatically reduces the possibility that radionuclides could be transported from the repository if a waste container fails.

Although the present-day characteristics of Yucca Mountain play an important role in assessing the suitability of the potential site, it is even more important to have the ability to simulate the potential repository's interaction with the natural setting over the repository's lifetime. We are using the massively parallel computational hardware being acquired by Lawrence Livermore to increase the reliability and accuracy of simulations designed to evaluate how such a nuclear waste repository will evolve over its prescribed lifetime of 10,000 years.

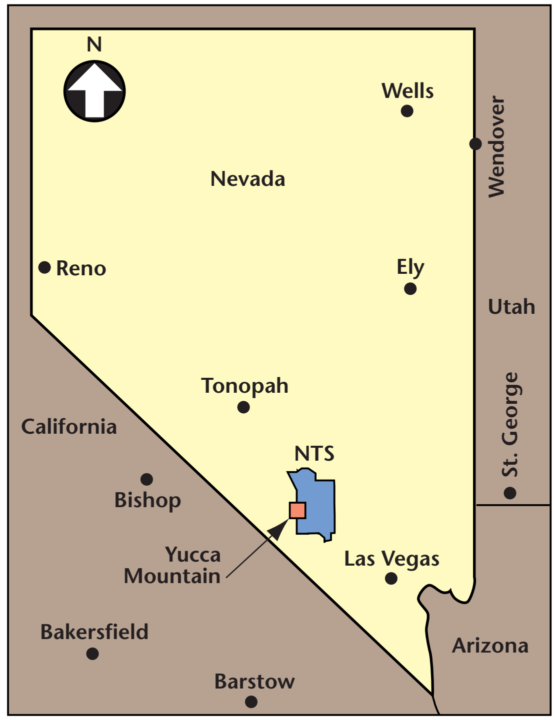

Figure 1. Yucca Mountain, located on federal land approximately 90 miles northwest of Las Vegas, Nevada, is composed of volcanic rocks that erupted 12 to 18 million years ago. Evidence suggests that the rock units composing the potential underground repository have always been above the water table.

The Concept of Reactive Transport and Coupled Processes

Although the rock that makes up the potential repository superficially appears to be

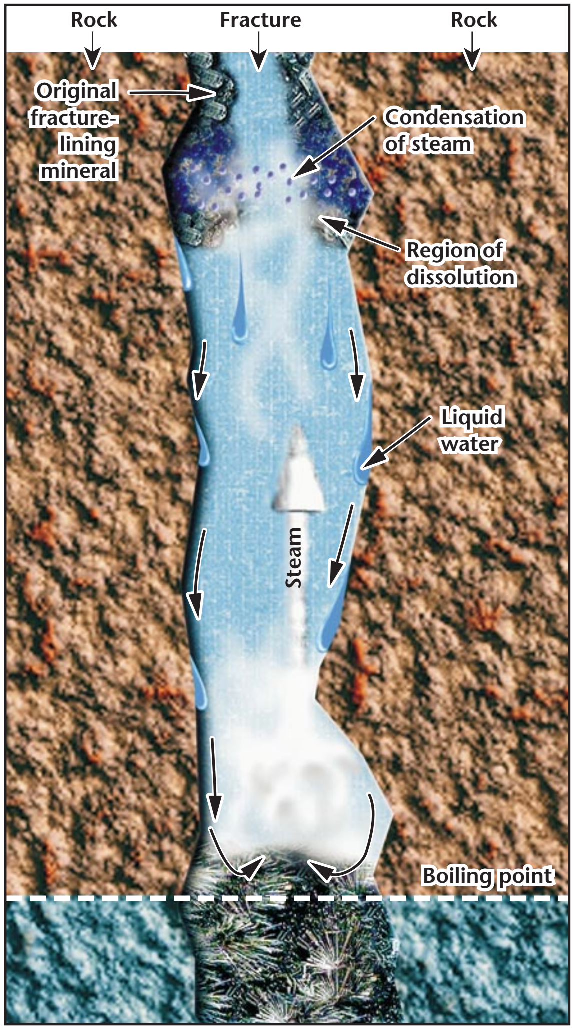

Figure 2. Conceptual model of reactive transport. Reactive transport occurs when liquid water chemically reacts with rock through which it is moving. Steam is generated in those regions where the temperature is at the boiling point. The steam migrates upward through fractures in the rock and condenses where the temperature is below the boiling point. This condensate, which is essentially distilled water, begins to dissolve any minerals that line the fracture, and continues to do so as it flows downward under the influence of gravity. It may also precipitate minerals as it flows, if concentrations of the dissolved elements become high enough (see Figure 3 for an example). If the water returns to the region where the temperature is at the boiling point, it again vaporizes, leaving behind minerals that then coat the fracture, forming a second generation of fracture-lining minerals. This process of dissolution in one region and precipitation of minerals in another can dramatically modify fracture geometry, leading to the formation of void spaces in one area and sealed fractures in another.

dry, the microscopic pores present in the rock contain a small volume of liquid water, which is a common feature of virtually all rocks. Since radioactive decay naturally generates heat, the radioactive waste emplaced in a nuclear waste repository will heat the enclosing rock and its associated pores. This heat will mobilize the enclosed pore water, which will tend to boil in the near vicinity of the waste, migrate away, and condense and accumulate in cooler areas.

Water is a weakly reactive liquid. When it comes in contact with rock, it slowly dissolves small quantities of the minerals composing the rock, and may precipitate other minerals if concentrations of the dissolved elements reach sufficiently high concentrations. As a result, the water that has moved in response to the waste heat slowly but progressively changes the size and distribution of pores and fractures through which the water may move. This process is termed *reactive transport* (Figure 2). The structures of pores and fractures are also modified by mechanical effects as the rock expands and contracts during the heating cycle. These changes, in turn, alter the rate at which water can move through the rock, by increasing or decreasing the cross-sectional area through which the water moves, and by changing the roughness of the surfaces the water contacts.

When taken together, these mechanical and chemical processes are coupled back to the movement of water, since they modify the properties that control water movement, such as pore and fracture dimensions and surface roughness. Thus, to realistically simulate the evolution of a repository requires the ability to calculate how these various feedback loops interact with each other over thousands of years. This becomes of great importance since these interactions determine where, when, and how much water may reach waste containers.

Reactive transport is also important for predicting the extent to which movement of radionuclides would occur if waste containers fail. Minerals that compose rock can retard movement of radionuclides dissolved

in water, either by exchanging elements in the crystal lattice of the mineral for the radionuclides, or by absorbing onto their surfaces the dissolved radioactive elements. The extent to which this occurs varies from one mineral to another, and from one radioactive element to another. Prediction of the extent to which radionuclides would migrate thus depends upon knowing the abundance and location of the specific minerals that would form along the flow pathways, and how these mineral populations change with time (Figure 3).

The Role of Massively Parallel Computers

In the past, our ability to accurately simulate reactive transport in natural systems has been constrained by limitations in available computational power. For example, to represent reactive transport in a complex geological system, such as a nuclear waste repository, it is necessary to represent the energy balance between the heat source, pore and fracture water that heats and possibly boils, air and steam, and rock. We must account for pressure changes as water and water vapor of different temperatures migrate through the complex geological units, ensure conservation of mass and momentum, honor the laws of thermodynamics, and account for the rates of mineral reactions. Evaluation of these and other interactions requires consideration of hundreds of independent chemical, mechanical, and physical variables at many millions of locations simultaneously. These calculations must be repeated hundreds to thousands of times, in order to complete a single simulation that includes the changes that occur progressively as the repository evolves through time.

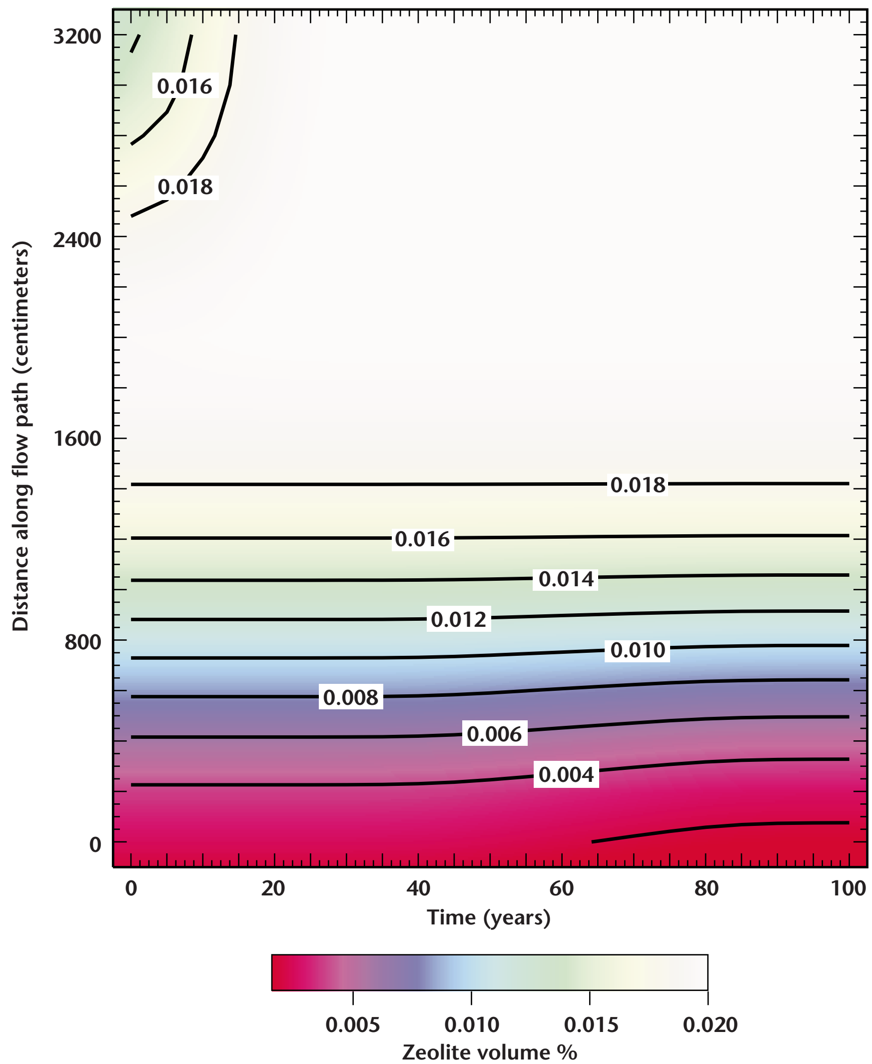

Figure 3. A model of the evolution of a sorptive mineral (in this case, a zeolite) along a fracture surface, after a 10-year period. The vertical axis indicates distance along the flow path, and the horizontal axis indicates the amount of time that has passed. The contours indicate how much zeolite has formed at each position along the flow path at the respective time on the horizontal axis. The zero point along the flow path is the point at which condensate first forms. Although the amount of mineral is small, it is sufficient to have a significant impact on the amount of radionuclides trapped on the fracture surface.

Such full-blown calculations are effectively impossible using modern computer workstations, because they contain, at most, a few processors that generally work serially. A single such calculation would require many years to complete on these machines. Many such simulations must be done to evaluate various “what if” scenarios for repository behavior. As a result of these limitations, much of the effort to date has been focused on developing methods for describing repository evolution using simplified models.

Recent advances in computer architecture have now made it possible to directly address the problem of simulating reactive transport and coupled processes, and have diminished the necessity to abstract and simplify. We are exploiting state-of-the-art massively parallel processor (MPP) architecture that is being acquired by Livermore as part of the Accelerated Strategic Computing Initiative (ASCI). The hardware that is coming online will allow computations to be conducted simultaneously on hundreds of very fast processors; the type of problem that was previously intractable because of its complexity can now be addressed. We are now constructing software that will utilize this hardware to simulate, with unprecedented resolution and accuracy, the coupled processes that will modify rock composing the potential repository.

Scientific and Computational Challenges

There are two facets to this challenge that need to be addressed simultaneously. One reflects the current state of knowledge regarding coupled processes in geological systems; the other stems from the new computational environment that is coming online.

Although most of the basic scientific aspects of this problem are well described mathematically, there are a number of processes for which rigorous mathematical descriptions remain a matter of debate. These issues include the mechanisms that operate at the atomic level that control the dissolution and precipitation of minerals, the absorption of metal atoms onto surfaces while in a solution that is moving, and the influence of changes in pore structure on the ability of liquids to move through them. The competing mathematical descriptions of these processes can be quickly tested using Livermore’s MPP capabilities, to determine the sensitivity of the outcome to the various models.

On the computational side, a number of challenges center around how best to structure computations in this unique environment. Strategies must be developed for efficiently coordinating computations among the many different processors. In addition, the body of data that will be generated by

these calculations is immense. A strategy must be developed for representing the data in such a way that they will be useful for both the scientists conducting the simulations (who need to visualize details of how the mountain may evolve), and the managers who must make decisions that are motivated by regulatory requirements.

To address these many issues, we are following a "rapid prototyping" approach in which a target problem is developed that exercises the basic capabilities needed for the complex problem, but which can be represented by a few variables in a simple way. This allows us to quickly test the model we are developing, progressively extend its complexity as we achieve success, and quickly sort out problems in our approach, without having to do this after all of the complexity has been built into the model.

Future Work

Demonstrating that the results obtained from such complex simulations are physically realistic is difficult, especially when one considers that we will be representing a future hundreds to thousands of years away. Fortunately, the Yucca Mountain Project has initiated a series of field experiments in which heat is being added to rocks that are identical to those that would be present in the repository. These experiments are designed to last years, and are sufficiently monitored so that changes can be sensed and evaluated. This important database will allow us to compare actual long-term responses to the simulations that we will conduct. In addition, a range of bench-top experiments and geological studies have been conducted which, although not as complete as the Yucca Mountain testing program, still provide an excellent database with which we can challenge the simulations. This validation effort will be the focus of our effort as development of the model proceeds.

The processes we are considering in these repository-specific simulations also take place in many other geological environments. The simulation capability we are developing can be used to understand the formation of ore deposits, the evolution and contamination of aquifers, the rate and mechanism for adding and removing elements from the oceans as sea-floor spreading progresses, and the evolution of oil and gas reservoirs. These are but a few of the applications this capability can address.

Expedited Demonstration of Molten Salt Oxidation Technology

Martyn Adamson, Peter Hsu, David Hipple, Kenneth Foster, Robert Hopper, and Timothy Ford

Molten salt oxidation (MSO), a promising alternative to the incineration process generally used to treat organic wastes before disposal, is a nonflame thermal treatment process. It completely destroys (oxidizes) the organic constituents of mixed wastes or hazardous wastes, including energetic materials, while retaining inorganic and radioactive constituents in the salt. ("Mixed" wastes are waste streams with both hazardous and radioactive properties.)

MSO technology is relatively mature, but to date has not been demonstrated as a fully integrated system for the treatment of low-level mixed wastes. "Integrated" means that the complete treatment train includes systems for the treatment of off-gas (gases produced during the process), the treatment of spent salt for reuse, and the preparation of robust (ceramic) solid final waste forms. In 1996, after cancellation of the Mixed-Waste Management Facility Project, Lawrence Livermore began preparations to expedite a smaller technology demonstration of molten salt oxidation using funding from the Department of Energy (DOE) Office of Environmental Management. The project combines chemistry and engineering expertise in the Earth and Environmental Sciences, Chemistry and Materials Sciences, and Engineering Directorates with the Laboratory's considerable experience in developing complex pilot-scale and demonstration systems. Our overall goal was to conduct a successful integrated demonstration of MSO, thereby demonstrating its efficacy for organic mixed-waste treatment and identifying for DOE the most suitable waste streams and waste types for MSO treatment.

The integrated pilot-scale treatment system was designed during the last half of 1996 and built during the first half of 1997. The MSO processor and off-gas system were activated in October 1997 and became fully operational in December 1997. Candidate low-level mixed-waste streams from DOE facilities are being identified. To date they include spent solvents, oils, and other organic liquids; plutonium-contaminated leaded gloves; spent ion-exchange resins; and spent activated carbon. The technology demonstration is also expected to be applicable to the treatment and disposal of a variety of medical and military wastes.

The Advantages of MSO

MSO technology is not new. Rockwell used the process more than 20 years ago for coal gasification, and they also demonstrated its effectiveness for destroying certain hazardous organics, such as PCBs and trichloroethylene. Extensive experience with laboratory-, bench-, and pilot-scale MSO units has been obtained at Rockwell, Oak Ridge National Laboratory, and Lawrence Livermore since the technology's introduction. Within the last five years, MSO also has been demonstrated as an effective method for destroying mixed waste oils and energetic materials.

Unlike incineration, in MSO the large thermal mass of molten salt provides a stable heat-transfer medium that resists thermal surges, ensures uniform temperature, and tolerates rapid process fluctuations. Flame-outs are completely avoided because MSO is a nonflame process that proceeds by catalytic, liquid-phase oxidation reactions. MSO generates less off-gas than incineration because it does not require supplemental fuel to sustain a flame. The MSO system operates at temperatures hundreds of degrees cooler than flame-combustion temperatures, which minimizes emissions of radioactive materials from mixed wastes. Acid gases are "scrubbed" by alkali salts, eliminating the need for a wet off-gas scrubbing system. These and related features are expected to be of benefit in the future permitting process for MSO.

The Livermore MSO Facility

Livermore's MSO facility (Figure 1) consists of several subsystems (Figure 2). The main components are a reaction vessel, an off-gas

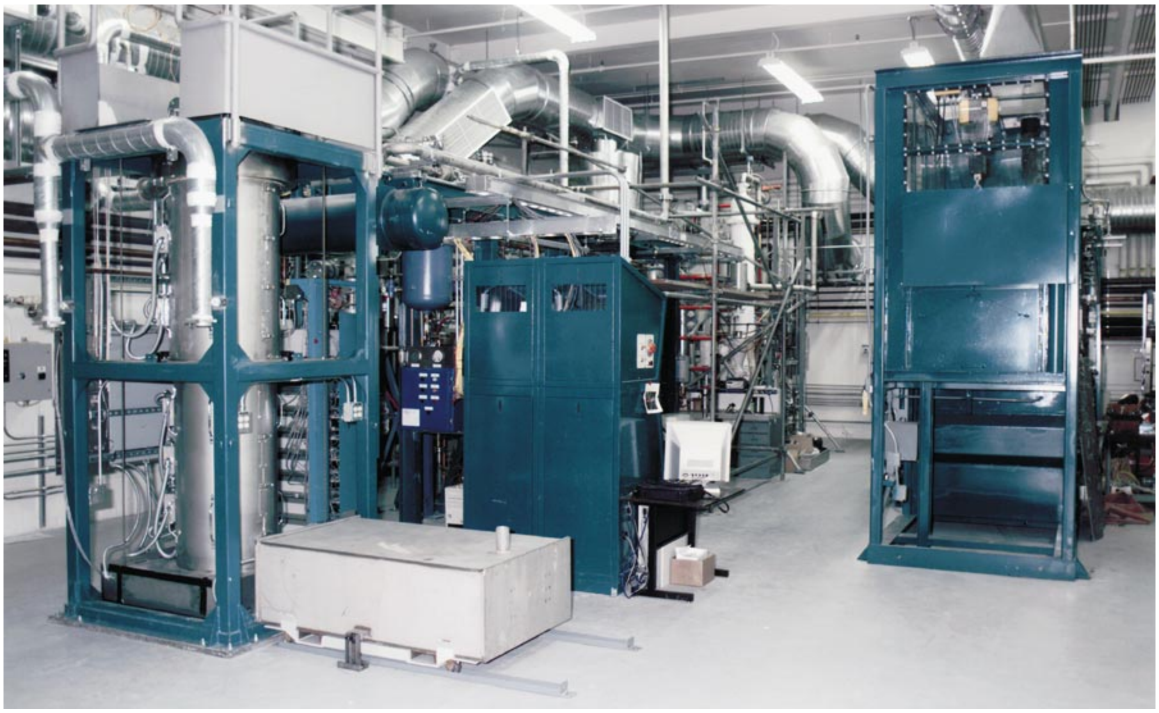

Figure 1. Livermore's new pilot plant for demonstration of molten salt oxidation: reaction vessel (left), instrumentation and control station (center), off-gas system (behind the vessel and the control station), and salt-recycle system (right). Equipment for preparing the final waste forms is out of view to the right.

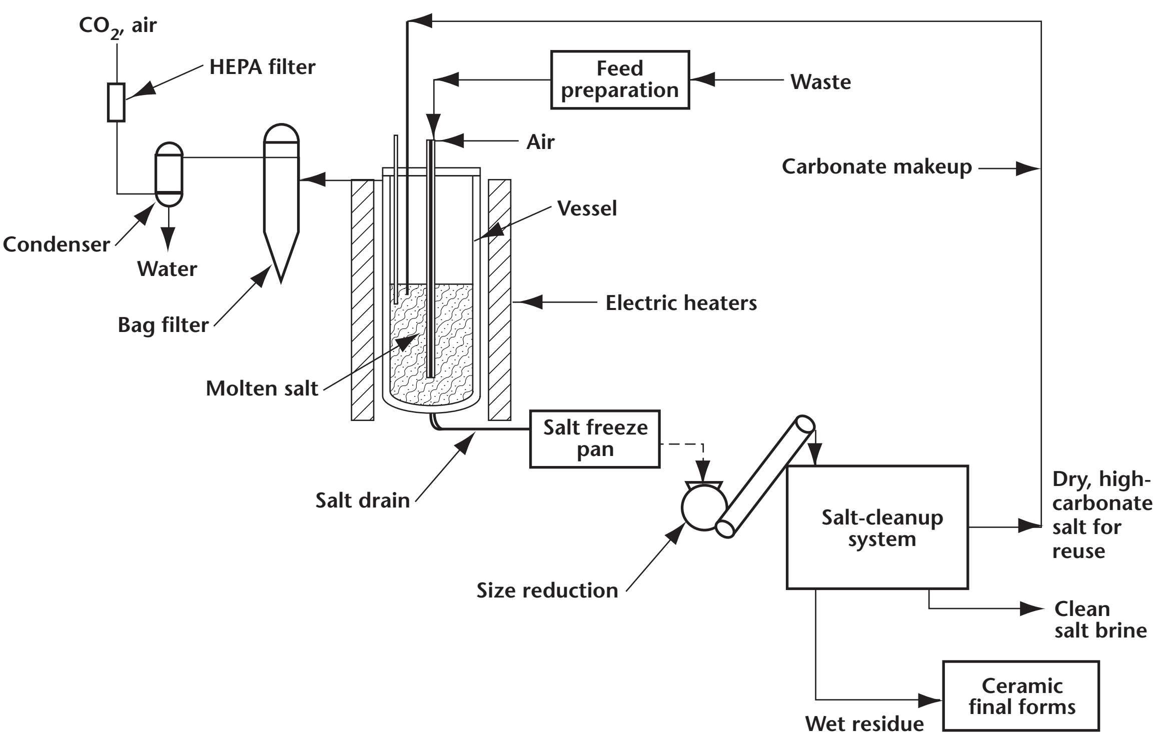

Figure 2. Simple schematic of the integrated MSO system.

treatment system, a salt-recycling system, feed-preparation equipment, and equipment for preparing ceramic final waste forms.

Plans for the facility include basic equipment for receiving waste, for separating solids and liquids, and for reducing the size of soft solid wastes, such as paper, rags, gloves, and booties. A metered supply of waste, or waste surrogate, is fed to the reaction vessel along with oxidant air using a top-feed injection system designed for both solid and liquid waste streams. Our present system can handle 2.3 kilograms (kg) of combustible solids per hour, or 7 kg of chlorinated solvents per hour. Organic-containing wastes are injected with excess oxidant air under a pool of molten carbonate salts at temperatures from 700 to 950°C. The normal salt load in the reaction vessel is 160 kg. The volume of the vessel above the salt level provides a disengagement zone for salt vapor and particles to separate from the off-gas before it exits. Flameless oxidation takes place within the salt bath, converting organic components of the waste into carbon dioxide and water.

Product gases exiting the vessel are treated in the off-gas system to remove any entrained salt particulates, water vapor, and traces of gas, such as carbon monoxide and nitrogen oxides (NO_x). Most of the entrained salt particulates in the off-gas are removed by a ceramic bag filter and water vapor is removed by a condenser. The off-gas then passes through a high-efficiency particulate air (HEPA) filter before going to a catalytic converter. The catalytic converter is designed to convert residual carbon monoxide (at parts-per-million [ppm] levels) into carbon dioxide in a catalyst bed at elevated temperatures. It is also equipped with an ammonia-injection system that converts NO_x into nitrogen and water by selective catalytic reduction. The off-gas leaving the catalytic converter is very clean and is exhausted to a building stack through a ducting system and another set of HEPA filters.

Halogens and heteroatoms, such as sulfur, are converted into acid gases, which are then "scrubbed" and trapped in the salt in forms such as sodium chloride and sodium sulfate. Other nonoxidizable inorganic constituents, heavy metals, and radionuclides are held captive in the salt either as metals or oxides, and most are easily separated—for subsequent disposal—in the salt-recycle system.

As residues of inorganic components build up in the salt bed, periodic removal of salt and replenishment with fresh salt is necessary to maintain efficiency. Many of the metals or radionuclides captured in the salt from real wastes will be hazardous or radioactive. Without further treatment, the removed spent salt would create a large secondary waste stream. Therefore, a salt-recycling system is used to segregate these materials, minimize the amount of secondary waste, and reduce the consumption of fresh salt. The segregated inorganic residues are encapsulated in a ceramic matrix for final disposal.

Experiments and Early Results

Off-Gas System

A smaller engineering development unit (EDU) was built in 1995 to verify MSO technology at an engineering scale before the integrated pilot-scale facility was built. We continuously monitored several species, such as oxygen, carbon monoxide, carbon dioxide, NO_x, and total organic carbon, in the off-gas during experiments. Concentrations of carbon monoxide and NO_x decreased as temperature increased. By measuring the ratio of total organic carbon in the feed to that in the off-gas, we found that the process efficiency was at or greater than 99.9999%.

In December 1997 we began experiments in our integrated MSO facility with several surrogate organic wastes, including toluene, mineral oil, ethylene glycol, pyridine, dimethyl sulfoxide, trimethyl phosphate, trichloroethylene, and Freon. An 8-hour test with toluene showed that total organic carbon in the off-gas was less than 1.0 ppm, an indication of very high process efficiency. The integrated system is now being equipped with sample collection trains for comprehensive analysis of off-gas species, including both volatile and semivolatile organic species.

Salt-Recycle System

The salt-recycle system receives spent salts from the MSO vessel and the off-gas system. The size of solidified spent salt chunks is first reduced in an enclosure before transfer to a tank in which the spent salt is dissolved in water. Most radioactive compounds coprecipitate with ash and mineral residue, and are removed from the salt solution after the first filtration step. Some radionuclides, such as thorium and uranium, form complex ions and stay in the solution. Our group has developed a process to remove uranium and thorium from salt solutions. The process, which includes pH adjustment, chemical reduction, and ion exchange, has been successfully demonstrated in lab-scale experiments.

This salt-recycling process was also demonstrated successfully with the EDU. Spent salt from EDU contained about 95 wt% sodium chloride along with minor amounts of several metals. Many of the metals were present at levels exceeding the Environmental Protection Agency (EPA) land-ban criteria, and such salt would be considered a hazardous waste if disposed of without further cleanup. Our salt-cleanup process was found to produce very clean, dry salt. Concentrations of metal species in the salt were mostly less than 100 ppm, and some were not detectable within the limits of our measuring techniques (Figure 3).

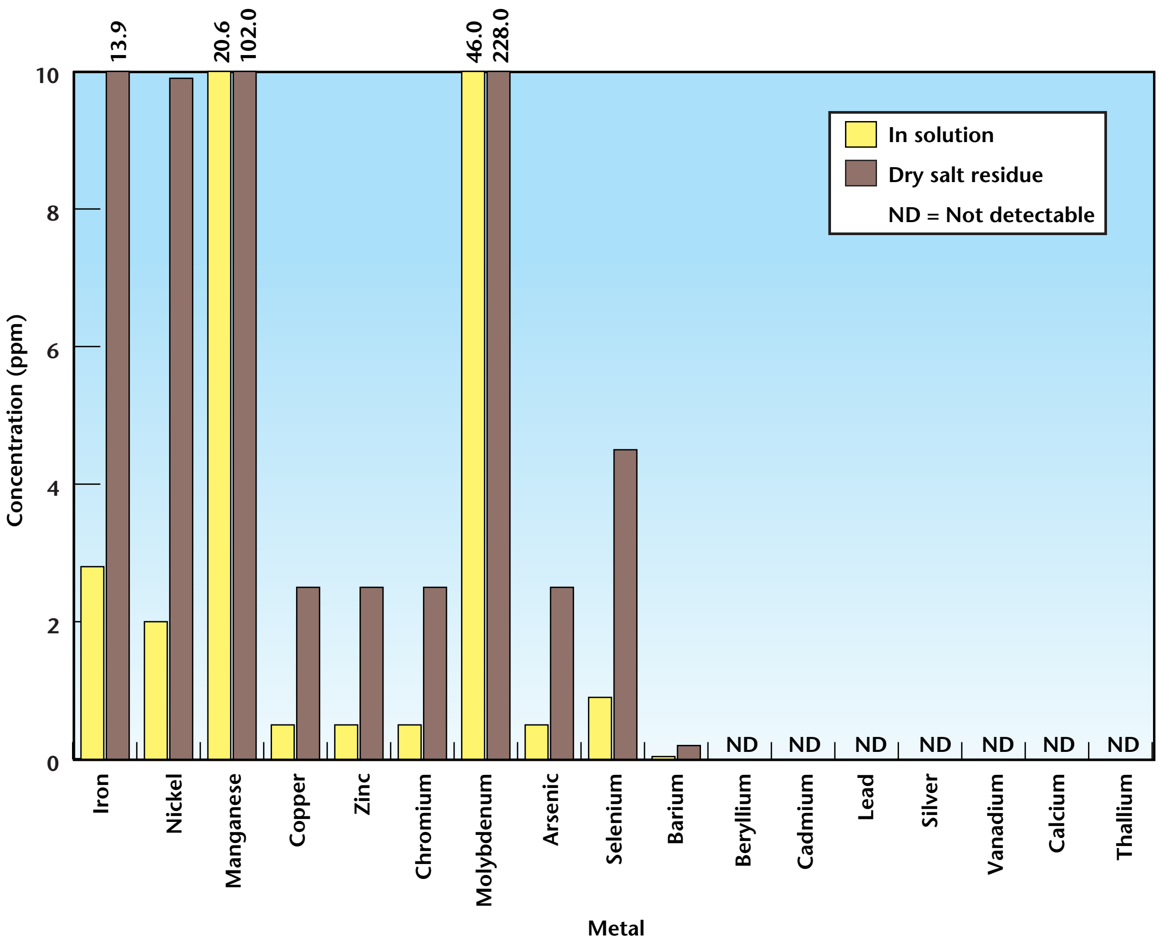

Figure 3. The salt-recycling process produces very clean, dry salt with low concentrations of key metal contaminants.

Ceramic Final Forms

Our recipes for ceramic final forms are designed to achieve maximum loading of inorganic residue into the ceramic form and to immobilize the mineral residues of the MSO system. Using bench-scale equipment, we fabricated more than 250 experimental ceramics under a range of processing conditions. They contain a wide variety of elements—as many as 46, including 15 of the 18 having leach limits assigned by federal or California regulations. These experiments are done to investigate phase formation, microstructure, partitioning, processing, and leach behavior. Resistance to leaching of regulated elements is generally excellent. Because the materials are rather complex, however, interpreting their properties is not simple.

We have characterized the experimental specimens by many different techniques, including gravimetry (to assess porosity), liquid-intrusion porosimetry (to study connected porosity), scanning electron microscopy (to examine microstructure and phase compositions), x-ray diffraction, x-ray fluorescence, electron microprobe, and other methods. A recent sample of our ceramic easily passed the original EPA regulatory limits for leaching, but barely failed newer and more stringent concentration limits for lead and vanadium. At least some of the lead and vanadium reside in the glass phase. We anticipate that future efforts to minimize residual glass will reduce the release of these elements.

Future Work

Ultimately, waste-treatment systems such as MSO technology will be tested to determine whether they can meet federal, state, and local treatment standards, residual product requirements, and effluent requirements. We expect that our MSO demonstration system will show that we can meet all Resource Conservation and Recovery Act (RCRA) Land Disposal Restriction standards, including Universal Treatment Standards for the chosen mixed-waste streams. The most favorable outcome of a successful demonstration is that MSO, together with its ancillary technologies, may be designated by the EPA as the best demonstrated available technology (BDAT), or its equivalent, for specified mixed-waste streams.

The integrated demonstrations performed through September 1998 will include destruction of a variety of organic liquids and organic solids on the order of 3 millimeters in size. Treatability studies will also be conducted in the facility with real low-level mixed-waste specimens during 1998. With knowledge and experience gained from this facility, safe and effective treatment of a variety of DOE mixed wastes and private-sector hazardous wastes should be possible. In seeking commercialization opportunities for the MSO technology, we plan to collaborate with other DOE sites that have specific and appropriate waste treatment needs, as well as with potential industry partners.

Transport and Fate of Chemical and Biological Releases in the Atmosphere

Don Ermak, Stevens Chan, Marty Leach, Bob Lee, John Leone, and Chuck Molenkamp

The Transport and Fate (T&F) effort is part of the Chemical and Biological Nonproliferation Program established by the U.S. Department of Energy to address the threat to national security posed by the proliferation of chemical and biological weapons. Drawn from Lawrence Livermore, Argonne, Lawrence Berkeley, and Los Alamos national laboratories, the T&F team is developing capabilities to support government response to potential attacks by urban terrorists using chemical/biological weapons. These capabilities will be applicable to preplanning and mitigation, real-time response, and post-event analysis and reconstruction. The team has two general goals: (1) to develop integrated and validated state-of-the-art modeling capabilities for the atmospheric transport and fate of chemical and biological agent releases within complex urban environments, and (2) to apply these modeling capabilities in a broad range of case studies to explore the range of probable consequences.

Selection of Models

The team's first task was to survey existing modeling capabilities for the various scales that are involved in chemical and biological releases in the urban environment (including identifying areas where research and development is needed to meet the T&F goals). Scale and physical considerations delineate four release scenarios of interest: (1) releases in a subway system; (2) releases within the interior of a building, including exchanges through multiple zones in the building; (3) exterior releases with contaminant dispersal around buildings and multi-building complexes; and (4) exterior releases with dispersal on the regional scale, from the urban area out into the suburbs and surrounding areas. The interior release scenarios include contaminant escape to the exterior and, conversely, the exterior release scenarios include infiltration into buildings.

The corresponding meteorological and dispersion scales are shown in Figure 1. Meteorological conditions on the regional scale are derived either from a diagnostic model, which produces a three-dimensional wind field that can be updated in time only when new observations are available, or a prognostic model, which forecasts the meteorological conditions using the time-dependent laws of physics. Models on the regional scale include the effects of variation in surface terrain height, but do not explicitly include buildings. Rather, they attempt to represent the effects of buildings using parameterizations and approximations.

An urban-scale model typically obtains its initial and boundary conditions, such as wind speed and direction, surface pressure and temperature, vertical profiles of temperature (or stability), and possibly the horizontal pressure gradient, from the regional scale. The model predicts flow fields around buildings and through street canyons, and differs from a regional-scale model in several important ways. For instance, the structure of one kind of model often differs fundamentally from that of the other because of the scale-dependent phenomena each is addressing. Urban-scale models must deal with the vertical faces of buildings, requiring a more complex grid structure, so they are often discretized more effectively using finite elements rather than finite differences. Also, representation of turbulence and other sub-grid processes requires different methods and approximations and, to date, moist processes are neglected in urban-scale models.

The urban models provide the boundary conditions for flow around individual buildings (building scale), which in turn provide information for flow within individual buildings

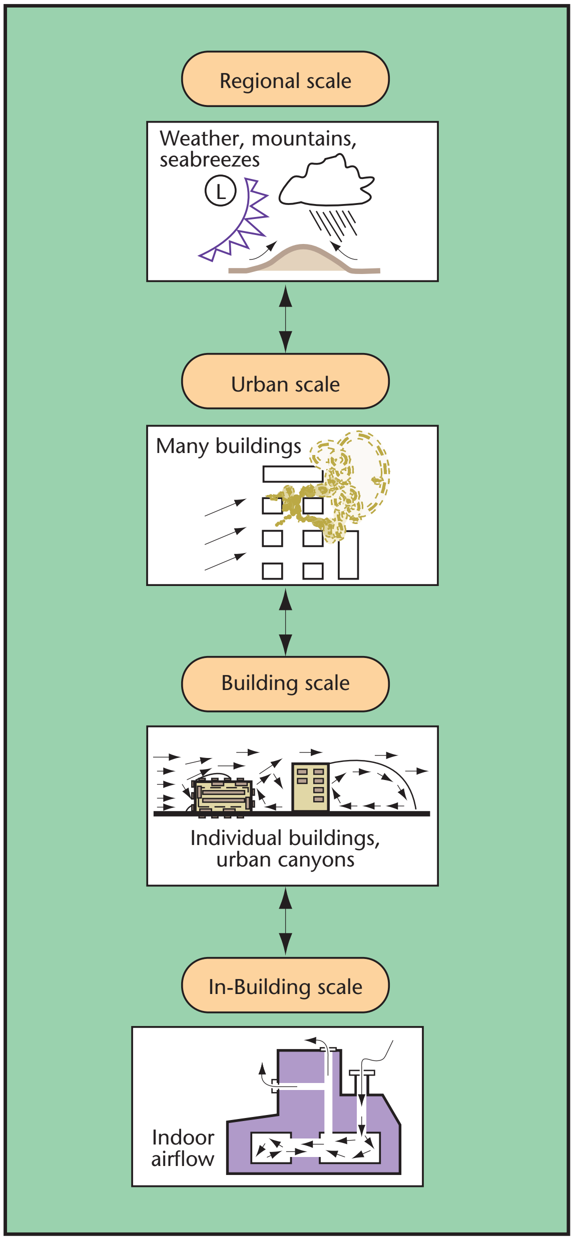

Figure 1. Predicting how chemical or biological weapons would be transported through the air after a release, and where they would end up, requires the interaction of models that address the problem at specific scales: regional (mesoscale), urban, building, and in-building. Livermore's Atmospheric Release Advisory Center, part of a multi-laboratory effort, is refining such models to support future U.S. response to potential urban terrorist attack.

or facilities such as subway systems (in-building scale). The information needs for flow around an individual building are similar to those for flow around an urban complex. To calculate the flow interior to a building, a new set of conditions is required. The pressure differentials on the exterior walls of the building can be obtained from the exterior models, but ventilation rates, heating and air-conditioning exchange rates, infiltration, and other individual building parameters must be specified.

Information transfers from larger to smaller scales when dealing with atmospheric conditions; that is, the larger-scale models provide the boundary conditions for the smaller-scale models. Information goes the other direction when a release occurs; a release of a chemical or biological agent is at the smallest scale (as a point, line, or area source), and the dispersion information passes up through the scales, providing the source term for the next-larger scale model.

The T&F team reviewed hundreds of models, including more than 20 that are available at the participating laboratories as well as models developed by other federal agencies, international cooperative efforts, private firms, and universities. The models selected for use by the T&F team cover the entire spectrum of scales including models for interior buildings and facilities, exterior buildings, urban complexes and areas, and regional studies.

The models were chosen to complement existing capabilities at the laboratories, specifically, those of Livermore's Atmospheric Release Advisory Center, which is the real-time incident-response capability planned for use in the Chemical and Biological Nonproliferation Program. Four of the chosen models are currently available at Livermore: FEM3C (individual building to urban scale—a prognostic flow field model with coupled dispersion), LODI (urban to regional scale—a dispersion model), ADAPT (urban to regional scale—a diagnostic wind-field model), and COAMPS (regional scale—a prognostic meteorology model).

Case Studies

The team is now focusing on using the models for case studies and scenario analysis. The case studies provide a baseline of the models' capabilities and limitations. For example, the FEM3C code was used to simulate the complex flow fields around a cubical building 60 × 60 × 60 meters in size (Figure 2). The building was assumed to be aligned with the direction of a uniform flow of 7 meters per second under neutral atmospheric conditions. Recognizing the symmetric property of the problem, we simulated only one-half of the flow fields in a computational domain of 480 meters (downwind) × 150 meters (crosswind) × 180 meters (height). The simulation used a graded mesh with slightly over 33,000 grid points and a minimum grid spacing of 2 meters in all directions. The calculated flow features are very consistent with published laboratory observations. Besides the flow around an individual building, FEM3C has also been used to simulate the flow around a complex of several buildings.

Case studies and scenario analyses also continue with the other models. LODI, a dispersion integrator, is linked to either ADAPT or COAMPS to provide transport and fate calculations at a somewhat larger scale. ADAPT, using observations of the winds and thermodynamic state of the atmosphere with simple physical constraints, creates a kinematic (varying in space but constant in time) view of the atmospheric flow. COAMPS, using those same observations with a more complete set of physical laws, creates a more dynamic view of the atmosphere that changes with time. These models are currently being used to study scenarios in areas with complex topographic forcing, such as the greater San Francisco Bay area.

Once the case studies are completed and the capabilities and limitations of the models are assessed, new capabilities will be added to the models. For instance, few of the models include chemical transformation, biological degradation, or particulate physics such as settling or resuspension. Inclusion of these processes in the models is needed to provide accurate simulations and consequence analysis of the impacts from potential chemical and biological terrorist releases in the urban environment.

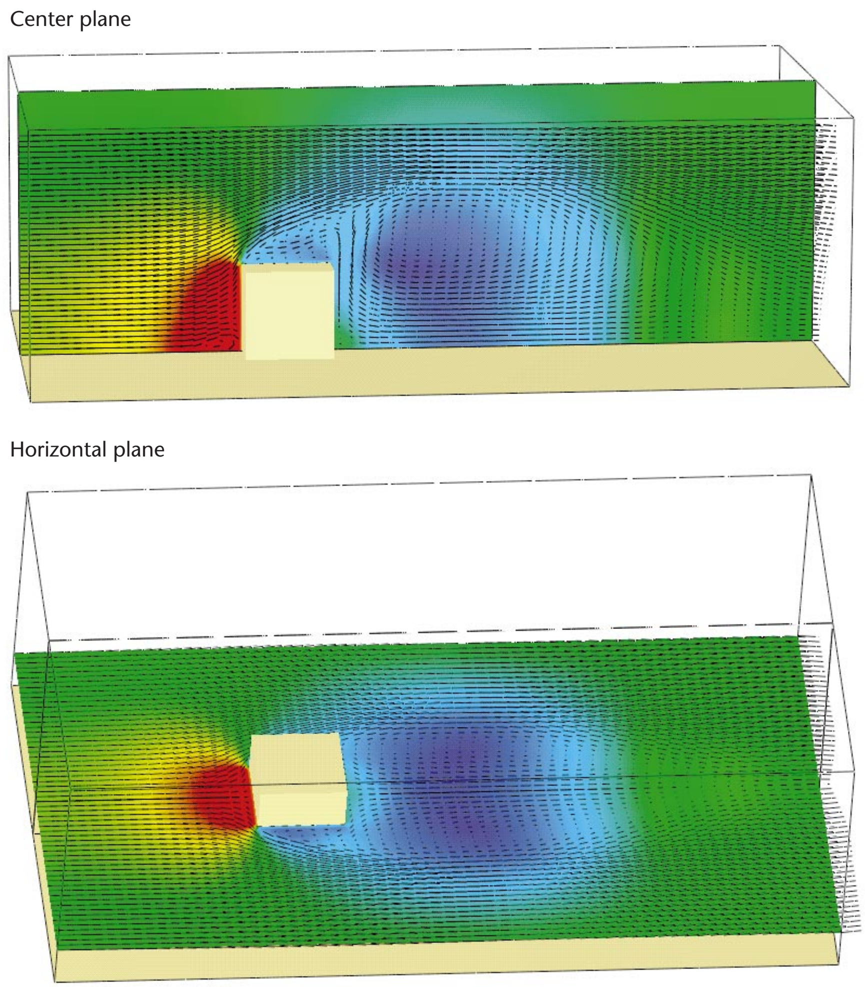

Figure 2. **A case study of the urban-to-building-scale model FEM3C used for a cubical building shows calculated velocity fields and pressures (red = high pressure, blue = low pressure) on two representative planes. The key features of the simulated results are flow separations, the recirculating flow (on the center plane), and a pair of rotating vortices (on the horizontal plane) in the wake of the building. Additionally, there are small eddies in front of the building and separated and reverse flow (but no reattachment) on the roof and sides of the building.**

The Timing of Earthquakes on the Northern Hayward Fault

John Southon

In 1990 the U.S. Geological Survey identified the northern Hayward Fault as the prime candidate (probability 0.28 in 30 years) for producing the next magnitude-7 earthquake in the San Francisco Bay Area. The fault passes through the heavily urbanized East Bay, directly under Berkeley's Memorial Stadium and the Warren Freeway, close to major hospitals and colleges, and runs as close to the Bay Bridge and the center of San Francisco as the better-known San Andreas Fault. A fair indication of the outcome of a magnitude-7 event on the northern Hayward Fault can be seen in the destruction from the recent earthquake in Kobe, Japan; its geologic setting and degree of urbanization are similar.

The recurrence estimate rests in part on the assumption, based on historical archives, that the last large event on this section of the fault occurred in 1836. However, recent reevaluation of the historical record by California state geologists suggests that the 1836 event was more likely farther south, perhaps as far away as Santa Cruz. This reinterpretation pushes the timing of the last major event on the northern Hayward Fault back, possibly before the 1770s, and throws doubt on the previous probability estimates.

Paleoseismic methods such as carbon-14 dating are used by geologists to determine the timing of surface-faulting events when historical records are missing or ambiguous. Scientists from Lawrence Livermore's Center for Accelerator Mass Spectroscopy and from the U.S. Geological Survey collaborated in 1997 to map strata in a section of the Hayward fault and perform radiocarbon dating. The results have major implications for Bay Area earthquake risk assessment.

Finding a Site for a Fault Trench

To date events on a surface fault, geologists examine suitable natural exposures, or the walls of trenches dug across a fault trace, for evidence of faulting: soil or sediment layers that are broken were laid down before the seismic event occurred, whereas overlying layers that are not broken were accumulated later. If both layers contain carbon-dateable material, such as wood, twigs, leaves, or charcoal from forest fires, then dates on samples from each can be used to bracket the time of the earthquake.

One difficulty in these studies is that faults in urban areas—where data on slip rate and recurrence rates are most urgently needed—are difficult to access. Most of the northern Hayward trace is inaccessible because it lies under structures, highways, and parking lots. Also, recurrence-rate studies require a site where sedimentation is regular and relatively fast, such as a pond or bog. (A site on rocky ground, or one where soil cover builds up very slowly, may be faulted but will not allow the details of successive events to be separated.) USGS geologists studied the small fraction of the northern Hayward Fault that can be reached (40–50 km), and found just four or five suitable sites.

One of these was a small depression on the second fairway of the Mira Vista Golf and Country Club, part way up the Berkeley Hills escarpment in El Cerrito. The depression is a small sediment-filled sag pond, formed where the two sides of the fault pulled apart. Two 10- × 40-ft trenches were excavated and U.S. Geological Survey scientists began detailed logging of the trench walls—mapping the strata and the faulting by drawing and by photomosaic (Figure 1).

Usually, such excavations are kept open for weeks or months. Small details of the stratigraphy become apparent over time as the color and texture of the sediments change as the trench walls dry out. Repeated visits to the site allow resolution of ambiguous interpretations of the trench logs. However, in this case time was extremely short. Permission had been given to open the trench for just 10 days, two

Figure 1. U.S. Geological Survey geologists map sedimentary strata in the walls of a trench dug across the Hayward Fault, in preparation for radiocarbon dating of faulting events by Livermore's Center for Accelerator Mass Spectroscopy.

of which would be spent refilling it to allow use of the golf course.

The walls of the trenches showed that this was indeed a good site. Multiple sediment layers were clearly visible, and there was no evidence of disturbances from erosion or from animal burrowing. Numerous terminations of vertical faults and disruptions of strata provided strong evidence for several seismic events. Several of the sediment layers contained abundant ash and charcoal fragments that allowed radiocarbon dating.

Radiocarbon Dating in Record Turnaround Time

Eighty small charcoal samples were brought back to Livermore for radiocarbon dating at the Center for Accelerator Mass Spectroscopy (AMS). AMS differs from the older counting methods of measuring radiocarbon, which detect the decay of carbon-14 atoms in the sample. Instead, AMS converts a fraction of the sample into a charged particle beam, and uses mass spectrometry coupled with nuclear physics particle-detection methods to separate the carbon-14 ions from other carbon isotopes and contaminants.

Because it is far more efficient than counting techniques, AMS is the ideal technique for studies that require the analysis of large numbers of small samples in a short time. Carbon sample sizes as small as 0.1 mg can be handled, and measurements take minutes rather than hours. The measurements themselves take only minutes, but the chemical pretreatment and sample preparation occupy several days or weeks, and turnaround times of weeks or even months are typical for radiocarbon dates.

For this study, for which time was critical, we began producing dates just 3–4 days after collecting samples from the trench site, for several batches of 20 or so samples. This fast turnaround provided a time scale for the site. Without this turnaround, the geologists would not have known whether the entire depth of the trench represented several thousand years of deposition or just a few hundred. Once the initial results were in, it was possible to resample and redate critical areas in the short time before the trench was closed.

Recurrence-Rate Results

The results showed that the 10-ft depth of the trench corresponded to about 6000 years of sedimentation. Initial interpretations of clusters of radiocarbon dates from strata above and below vertical fault terminations suggested that at least four surface-faulting events occurred in the past 2250 years BP (Before Present): two between about 2250 and 1430 BP and two more after 1170 BP. However, further analysis has pinpointed additional signs of faulting, indicating that 7 events (and perhaps as many as 9) occurred in this time period. This revised interpretation is much more consistent with previous recurrence-rate estimates of 170–200 years.

This study highlights the paucity of information about recurrence rates for large events on Bay Area faults, and some of the difficulties in obtaining such information. Because a large event on one fault may increase or decrease the stress on others, the relatively short historical record of movements on Bay Area faults may give a distorted picture. Trenching studies are essential for a longer-term perspective, and as this study suggests, investigations at multiple sites on any given fault may be necessary to capture the full details of the record. Paleoseismic studies have been carried out or are currently taking place on other Bay Area faults besides the northern Hayward Fault, and a major expansion of this kind of work is expected in preparation for the upcoming 1999 Bay Area Earthquake Probability Update.

Resettlement of Bikini Atoll—A Former U.S. Nuclear Test Site

William Robison and Terry Hamilton

Bikini Atoll is one of two sites in the Marshall Islands that were used in the 1950s by the United States for testing nuclear weapons. The CASTLE–BRAVO test in 1954 produced widespread radioactive contamination over much of the northern Marshall Islands (Figure 1). The Bikini people, relocated in 1946 before the test program began, have long desired to return to their homeland. Cleanup and planting of food crops began in 1968, followed by limited resettlement in 1970. However, dose estimates made later by Lawrence Livermore, and confirmed by Brookhaven National Laboratory, indicated that when locally grown crops matured and became available for consumption, the resulting body burden of the radionuclide cesium-137 and the associated dose would exceed federal guidelines (Robison et al., 1977). In August 1978, the reestablished residents on Bikini Island had to be relocated again.

Under the auspices of the U.S. Department of Energy, the Health and Ecological Assessment Division at Lawrence Livermore plays a key role in providing data and assessments to assist atoll communities with making informed decisions about resettlement options. Our long-term mission is to ensure the safe resettlement of the four affected atolls—Bikini, Enewetak, Rongelap, and Utirik.

Cesium-137 Transfer from Soils into Plants

Marshall Island coral soils—especially on Bikini Island—make cesium-137 much more available for plant uptake than do soils of North America and Europe. Soil-to-plant

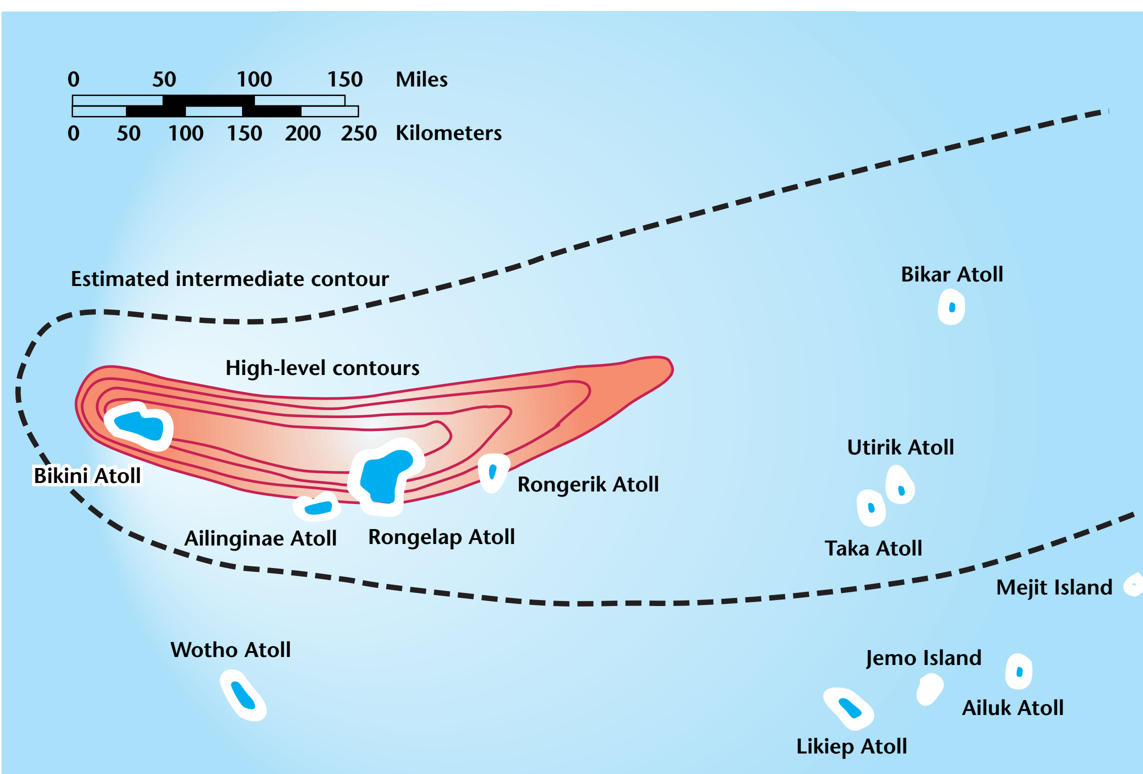

Figure 1. Map of the Marshall Islands, showing the location of the Bikini Atoll and the fallout pattern from the CASTLE-BRAVO nuclear test of 1954.

cesium-137 transfer factors (becquerel per kilogram dry weight plant/becquerel per kilogram dry weight soil) for tropical fruits on Bikini Island range between 2 and 40. This compares with values between 0.005 and 0.5 for vegetation growing in temperate zones (IAEA 1994).

This very significant difference occurs because coral soils are composed almost entirely of calcium–magnesium–strontium carbonate with varying amounts of organic matter, essentially little or no aluminosilicate material, and very low concentrations of potassium. Enhanced plant uptake of cesium-137 on Bikini Island can be attributed to both the absence of clay mineral binding sites and the low concentration of potassium in the soil. Knowledge of preferential uptake of cesium-137 into local food crops was a major factor in (1) reliably predicting the dose for returning residents, and (2) developing a strategy to limit the availability and uptake of cesium-137 into those crops.

Dose Assessments

We recently completed a detailed dose assessment for Bikini Atoll assuming a resettlement date of 1999. Doses were estimated for all exposure pathways and compared with background doses to assess the need for and consequences of control measures. The dose was calculated using radionuclide data for cesium-137, strontium-90, plutonium-239 and -240, and americium-241 in locally grown foods, a diet model for pertinent local food consumption, external gamma exposure calculations, and exposure via inhalation from radionuclide resuspension. We estimate that the ingestion pathway will contribute 90% of the dose to returning residents, mostly through uptake of cesium-137 into terrestrial foods such as coconut, *Pandanus*, breadfruit, and papaya (Robison et al., 1997).

External gamma exposure from cesium-137 accounts for about 10% of the dose. Plutonium-239 and -240 and americium-241 are major contributors to the dose via inhalation, but this pathway contributes only about 1% of the total.

The estimated maximum annual effective dose due to weapons testing for current Bikini Island living conditions is about 4 millisieverts per year (mSv/y) when imported foods are available. The natural background dose in the Marshall Islands is about 2.4 mSv/y, of which a significant fraction comes from consumption of fresh fish. The estimated background dose plus the bomb-related dose totals 6.4 mSv, which exceeds the average background doses of 3 mSv/y in the U.S. and 2.4 mSv/y in Europe.

Guidelines for controlling prospective dose to the general public (from nuclear power plants, for example) are not relevant to situations where people want to resettle in areas contaminated by nuclear weapons fallout. General guidance provided by the International Commission on Radiological Protection and the International Atomic Energy Agency recognizes that below an effective annual dose of 10 mSv, the situation should be reviewed, and if a cost-effective, socially acceptable, and environmentally sound remediation strategy can be implemented to reduce the dose, it should be considered. Our goal is to develop cost-effective measures to reduce the dose associated with resettlement at the atolls.

Remedial Measures to Reduce Doses

An effective method to reduce the island radionuclide inventory is to remove the organic-rich layer of soil that extends to about 40 cm depth; much of the cesium-137 is retained within this layer. This material, derived largely from litter from surrounding vegetation, supplies nutrients for plant growth and controls the water-retention and cation-exchange capacity

of soil. Consequently, its removal leads to severe environmental impacts that require very-long-term commitments to rebuild the soil and revegetate the island.

We have evaluated several other measures to eliminate cesium-137 from the soil and/or reduce its uptake into food crops. The most effective, and the easiest to implement, is the application of potassium to the atoll soils. A dramatic reduction in cesium-137 uptake occurs in tropical fruits after a single application of potassium-rich fertilizer to selected experimental plots on Bikini Island (Figure 2). This treatment reduces the associated ingestion dose to about 5% of pre-treatment levels. This option avoids soil removal, and the added potassium increases plant productivity.

The estimated dose for a resettlement scenario on Bikini Island where the top 25 cm of soil is removed in village and housing areas and the rest of the island is treated with potassium fertilizer is 0.41 mSv/y (compared with 4 mSv/y using no countermeasures); the 30-, 50- and 70-year integral doses are 9.8 mSv, 14 mSv, and 16 mSv, respectively. With this treatment, the average background effective dose over a 50-year period for the Marshall Islands would be about 120 mSv; in the United States it is 150 mSv. Hence, the background dose plus the nuclear fallout component at Bikini over 50 years is estimated to be less than the background dose in the United States.

Moreover, rainfall transports cesium-137 (and potassium) out of the root zone of plants into the groundwater. In the longer term this will lead to a reduction in cesium-137 levels in local food crops and reduce the current dose estimates even further. We are now focusing on determining the duration of the effects of potassium treatment on cesium-137 uptake into plants, and the rate of environmental loss of cesium-137 in the atoll ecosystem.

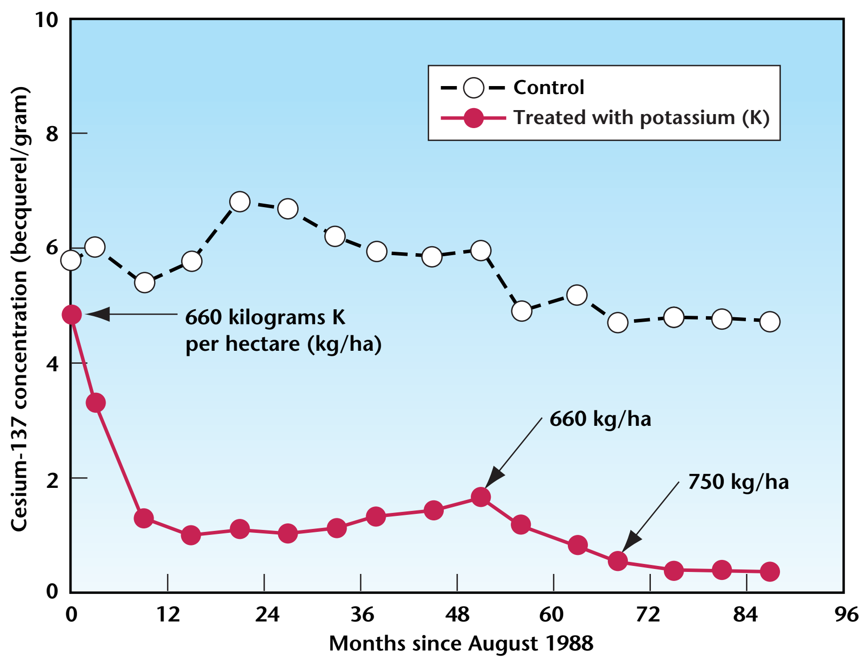

Figure 2. Effect of potassium treatment on the concentration of cesium-137 in coconut meat. The availability of potassium ions—an essential nutrient for plants—blocks the uptake of cesium-137 into the fruits, giving people resettling contaminated atolls an alternative to excavation of the topsoil and destruction of existing plantings of coconuts and other food crops. Our "combined option" recommends removal of soil in housing and village areas where people spend most of their time, in order to reduce the external dose, and treatment of the rest of the island with potassium fertilizer.

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Tiltmeter for Monitoring Deep Oil Wells

Steven Hunter and Carl Boro

Producing oil from American oil fields today involves more than simply sinking a well and waiting for a "gusher." More than half of our oil production requires help, usually in the form of fracturing the underground rock to provide channels through which oil can flow, thus increasing the well's oil production. This "hydrofracturing" is done by pumping a mixture of water, polymers, and sand down a well under high pressure. Hydrofracturing causes the surrounding rock to move slightly—enough that an array of ultra-sensitive tiltmeters emplaced near the surface may detect the slight tilting of the ground. The tilting at the surface reveals the primary direction of the cracking several thousand feet below. This information helps drillers decide where to sink additional wells.

The deepest hydrofracture that could be monitored with previous near-surface tiltmeters is 6000 ft. At Lawrence Livermore we have developed an instrument that increases the depth to at least 10,000 ft and allows us to monitor nearly five times as many wells. Deep wells cost much more than shallow wells, so the dollar value of the wells that can now be monitored is at least 20 times the dollar value of the wells that could be previously monitored. For the first time, oil companies will be able to get the fracture orientation for their very expensive deep wells; this is extremely valuable information for planning the locations of new wells.

How Tiltmeters Work

When tiltmeters are used in oil fields to detect the cracks from hydrofracturing, the tilt data from each tiltmeter are used to define the tilt vector's magnitude and direction at that site. The tilt vectors from an array of about 20 instruments are used to generate a map of the surface deformation around the oil well. A modeling program derives the hydrofracture direction that must be present to produce the observed tilt vectors.

Tiltmeters work on the same principle as a carpenter's level. The sensor is a liquid-filled glass tube with a gas bubble in the liquid. The tube contains electrodes so that circuitry can detect the position of the bubble. When the instrument is tilted, the position of the gas bubble shifts, and this shift causes changes in the impedance between two output electrodes and a common electrode. The tilt sensors need to be leveled to within a few milliradians for the sensors' output to be linear. This can be achieved by manually leveling the instrument during installation or by using motors to level the sensors within the instrument.

The tiltmeters need to be placed below ground because of the tilt "noise" at the surface. Natural sources of tilt noise include wind, thermal expansion of the surface, expansion due to hydration when it rains, and the tidal effects of the moon and the sun. Man-made sources of surface tilt noise include vehicle traffic and well pumps. Once the instruments' emplacement depths exceed 20 feet, however, manual leveling becomes impractical. Also, at that depth, surface noise can still affect ground tilt and interfere with signals coming to the tiltmeters from the deeper hydrofractures. Previous instruments had depth limitations because of emplacement techniques, or because of the electrical noise pickup that analog signals are susceptible to when they are sent to the surface over long wires to be digitized and stored.

The New Tiltmeter

The surface noise decreases with depth, so we designed our instrument to be deployed

deeply enough that the weak signals from very deep hydrofractures would be larger than the noise from surface sources. Our tiltmeter greatly expands the range of emplacement depths for which an adequate signal-to-noise ratio can be achieved (Figure 1).

To enable the instrument to be economically deployed at the 40- to 100-ft depths needed for imaging fractures deeper than 6000 ft, our redesign incorporates "slimhole" technologies, remote tilt-sensor leveling, an electronic compass for instrument orientation, a downhole analog/digital converter to reduce electronic noise, an internal data logger with a large memory, and low-noise analog electronics. In addition to gains derived from the improved signal-to-noise environment, the self-contained slimhole tiltmeter benefits from the more stable hole conditions that result when instruments are installed in smaller boreholes (3–5 inches in diameter).

This instrument includes motors to level the sensors within the instrument, both at installation and at any time that the tilt exceeds a maximum threshold—for instance, as subsidence occurs as oil is produced. The built-in data logger controls the motors and records the fact that releveling has occurred, so no external control box is necessary. As soon as power is applied, the instrument levels the sensors and starts acquiring data.

Advantages for Oil Production

Our new tiltmeter images hydrofractures that could never be imaged before. Only 20% of the oil wells in the United States are less than 6000 ft deep—the measurement limit of previous technology. Since we can now image deeper wells, nearly five times more wells can be imaged than with the old instruments.

More important than the increase in the number of wells that can be imaged is the economic impact of the increased measurement capability. The cost of drilling a 10,000-ft-deep oil well is far greater than twice the cost of drilling a 5000-ft-deep well. A 10,000-ft-deep well costs at least $1,000,000 and could cost much more if problems develop during the drilling. Therefore, the dollar value of the oil wells that can be imaged with our new instrument is more than 20 times the dollar value of the oil wells that could be previously imaged.

More than half of all the oil- and gas-production wells drilled in the United States depend on hydraulic fracturing to sustain or enhance their production. Precise knowledge of the principal hydraulic fracture orientations is essential for optimally placing vertical wells when drilling additional wells in a known oil field. Using data provided by the new tiltmeter, additional wells can be placed so that each well can produce the maximum

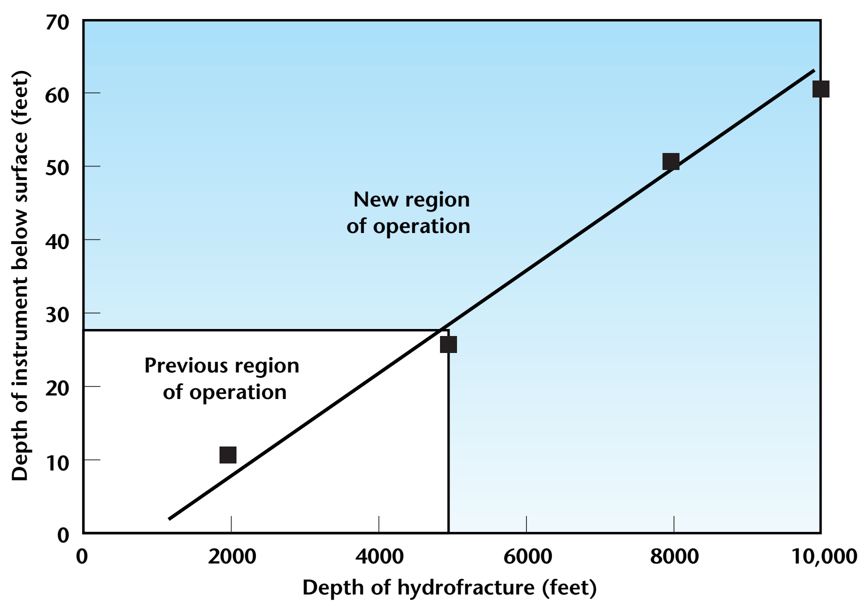

Figure 1. The new tiltmeter developed at Lawrence Livermore allows monitoring of oil-field hydrofracturing at much greater depths than before.

amount of oil, without interfering with adjacent wells (Figure 2).

This work should also provide improvements to tiltmeters used for earthquake and volcano research; we are in contact with scientists at the U.S. Geological Survey regarding such applications.

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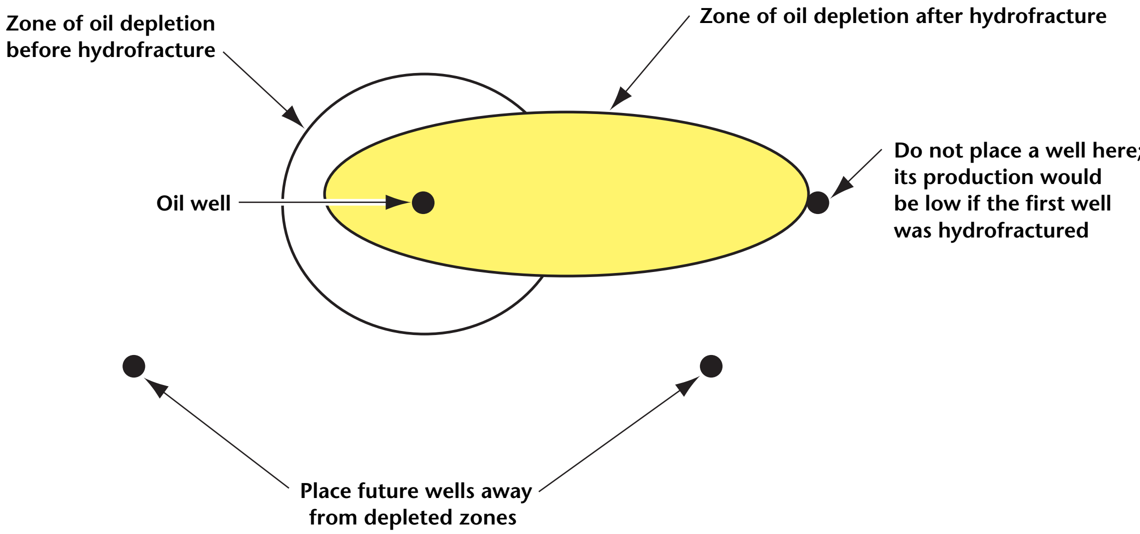
Figure 2. Using data provided by the new tiltmeter, new oil wells can be placed so that each well will produce a maximum amount without interfering with adjacent wells.



Containment of Sub-Critical Experiments for the Stockpile Stewardship and Management Program

Norman Burkhard

With the cessation of underground nuclear testing, the U.S. Department of Energy has put into action a far-reaching plan to ensure that the nation's nuclear force remains safe, secure, and reliable without new weapon development or the use of underground testing. This plan, the Stockpile Stewardship and Management Program (SSMP), will use enhanced computational and experimental capabilities to help predict, detect, evaluate, and correct problems affecting nuclear weapons in the national arsenal without additional nuclear testing. Stewardship of the U.S. nuclear stockpile is now Lawrence Livermore's "foremost responsibility," according to Livermore Director Bruce Tarter.

In the absence of nuclear testing, computer simulation is the only way to assess the performance of a complete nuclear weapon system. Numerical simulation also provides an essential tie to data from past nuclear tests and is an important means of predicting the performance and changes that might occur in the stockpile due to aging, environmental exposure, material incompatibilities, or other factors. In order to adequately model the performance of a nuclear weapon system on a computer (in the absence of actual testing), the material properties of various components and especially of the special nuclear material (SNM) in the nuclear weapon must be better known. In order to obtain this information, the SSMP is conducting a series of sub-critical zero-yield dynamic experiments. In these experiments, small high-explosive charges are used on sub-critical experiments to shock small quantities of SNM; diagnostics instrumentation measures properties of the SNM that are required for computer simulations of nuclear weapon systems.

These experiments are being conducted at the U.S. Nevada Test Site by the Nevada Experiments Program (N Program) of the Defense and Nuclear Technology Directorate. The authorization letter from the Department of Energy for sub-critical experiments requires that the Laboratory assure that no SNM will be released to any uncontrolled environment. The Containment Program residing in the Earth and Environmental Sciences Directorate and run for N Program is responsible for developing and fielding containment plans for the experiments.

Containment Plan for the HOLOG Experiment

During 1996 and most of 1997, the Containment Program developed and fielded the containment plan for the first Livermore sub-critical experiment, named HOLOG. (The name HOLOG was chosen because one of the physics experiments included the collection of holographic images of the ejecta from SNM when it had been shocked.) The containment plan for HOLOG was specifically developed for the location of the experimental testbed at NTS.

The experiments are being fielded in the U1a complex at the NTS, a network of tunnels and drifts approximately 1000 ft underground beneath the Yucca Flat area. A large vertical shaft is used to access the complex.

The containment plan developed for sub-critical experiments in the complex takes into account the specific geologic setting and the unique physics diagnostics requirements of the experiments. The U1a complex is mined in mixed alluvium about 500 ft above the standing water level. The drifts and tunnel are dry, enabling the construction of modern sophisticated physics laboratories underground. The alluvium is quite porous (gas-filled porosity is about 15 volume %) and permeable to gas flow (gas permeability is about 1.5 darcies).

An experimental chamber was built in an alcove off a drift in U1a (Figure 1). The alcove walls were covered with fibercrete and a paint that forms an elastomeric membrane. Recording stations outside the experimental chamber received experimental data via electrical and fiber-optic cables and direct optical lines-of-sight; the optical diagnostics required short optic-path lengths. Thus the containment barrier that sealed the alcove forming the experimental chamber had to be thin, include high-quality glass optical viewing ports, and be robust enough to contain the SNM within the chamber after the high-explosive detonation. A steel and fibercrete containment barrier with three viewing ports, anchored to the formation by a grout keyway system, was designed and constructed.

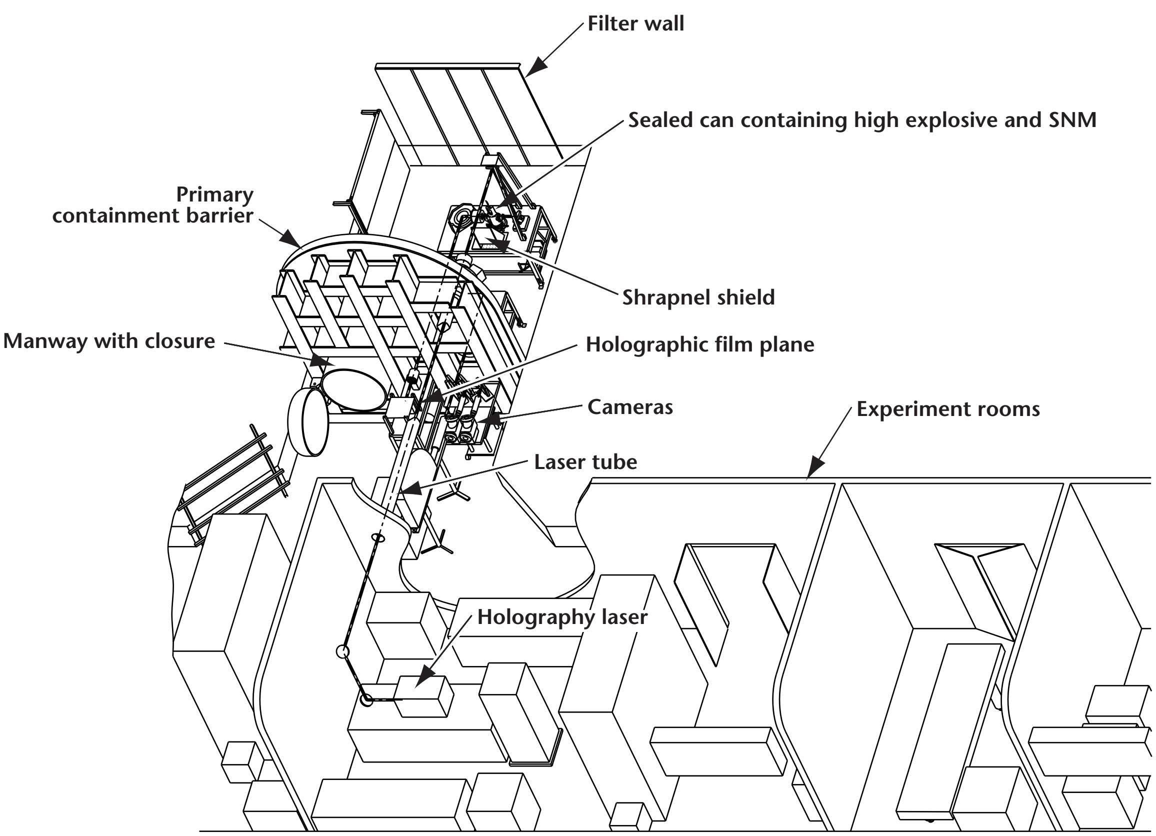


Figure 1. **Layout of the HOLOG experimental chamber in a tunnel drift at the Nevada Test Site. The primary containment barrier is constructed of steel and fibercrete. The alluvium surrounding the chamber acts as a high-efficiency particulate filter under porous-flow conditions, allowing complete containment of nuclear materials.**

A filter wall at one end of the chamber provided the main route for porous flow out of the chamber. Figure 1 shows the HOLOG experimental chamber and some of the physics diagnostics.

The containment plan developed for HOLOG (and for future LLNL sub-critical experiments in U1a) uses this alluvial setting to maximum advantage to meet the needs of the Department of Energy to protect the uncontrolled environment and to protect the expensive physics diagnostics equipment, which is only several feet from the experiments. Our containment goal on HOLOG was to contain all SNM within the experimental chamber or in the "skin" of the alluvium surrounding the chamber. The alluvium surrounding the experimental chamber allows the high-explosive gas products from the sub-critical experiment to porously flow from the chamber.

Successful Containment in Alluvium

Tests conducted using surrogate materials and SNM have shown that the alluvium in U1a acts as a very effective high-efficiency particulate accumulator (HEPA) filter for the SNM. The sub-critical experiment converts some of the SNM into an aerosol and particulates. No volatile SNM compounds are formed in U1a sub-critical experiments that could be transported through the alluvium. There are no known actinide organo-compounds with high enough vapor pressure at room temperature to migrate through the alluvium.

Pressure tests of the HOLOG experimental room were interpreted to provide the alluvial properties that affect porous flow. These parameters were then used to study the distribution of high-explosive gas following the execution of the HOLOG experiment on September 18, 1997.

Figure 2 is a comparison of the measured and predicted pressures in the experimental chamber after the HOLOG experiment. The measured data agree quite well with the calculated porous-flow data, suggesting that flow from the experimental chamber was purely porous flow. This was the desired result, since the tests with surrogate material had indicated that the alluvium would be an effective HEPA filter for SNM under porous-flow conditions.

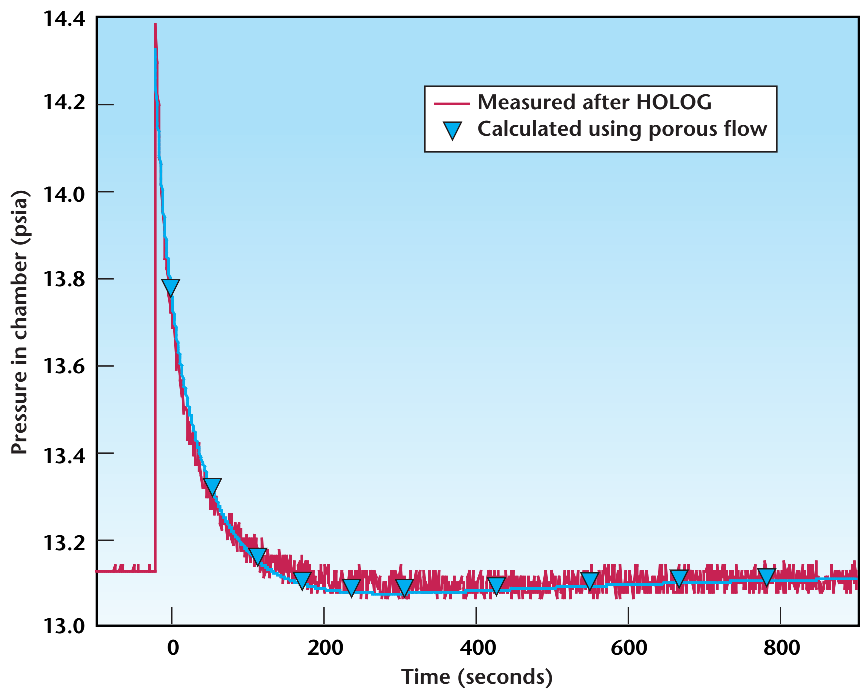


Figure 2. Measured and predicted pressures in the chamber after the HOLOG experiment. The agreement of the data indicate that flow from the experimental chamber was purely porous flow.

After the experiment, containment was evaluated by looking for SNM outside the experimental chamber in the drift of the U1a complex. All alpha-particle radiation detectors outside the experimental chamber remained at pre-shot background levels. Many swipes were taken around the HOLOG containment barrier and in the physics diagnostics room; no evidence was found that any SNM was released into the U1a complex or to any uncontrolled environment.

We are now constructing the experimental chambers for the next two Livermore sub-critical experiments. Mining and construction are well under way at U1a. The containment plan for these experiments follows the plan developed for HOLOG.

Star In a Jar: A New Model for Single-Bubble Sonoluminescence

William Moss, Douglas Clarke, and David Young

Sonoluminescence (SL) is a process in which sound waves aimed at a container of water nucleate, grow, and collapse many gas-filled bubbles to create ultrashort light flashes representing a trillionfold focusing of the initial sound energy. SL was discovered in 1933, but the phenomenon could not be studied in detail until 1990, when Gaitan (Gaitan, 1990; Gaitan et al., 1992) at the National Center for Physical Acoustics successfully obtained SL from a single air bubble. Lawrence Livermore scientists have developed a new theoretical model for single-bubble sonoluminescence (SBSL) that for the first time is consistent with experimental results and makes predictions about the sensitivity of SBSL to various parameters. The light-emitting regions of the bubble are similar to those in a miniature star; our new model provides insight that may be applicable to fusion-energy research.

The Sonoluminescence Phenomenon

In single-bubble sonoluminescence, sound waves levitate and trap a single micron-sized gas-filled bubble while forcing it to undergo SL repetitively. A bubble of air undergoing SL appears electric blue in color to the naked eye. Using Gaitan's methods, experiments at UCLA (Barber and Putterman, 1991) showed that SBSL from an air bubble produces light flashes that are synchronized with the periodically expanding and compressing sound field. Each flash had a measured duration less than 50 trillionths of a second, or 50 picoseconds (ps). The light flashes produced a spectrum of colors consistent with the idea that the sonoluminescing bubble has a temperature of at least 23,000 K.

These results created a scientific stampede in which experimentalists obtained more data and theorists tried to explain the data, especially the mechanisms underlying the ultrashort flashes and high temperatures of the bubble. Scientists proposed exotic mechanisms such as quantum vacuum fluctuations, fractoluminescence, and charged-liquid-jet collisions. Earlier, Jarman (1960) had suggested that the collapsing bubble generates an imploding shock wave that compresses and heats the gas in the bubble. Although work by Lawrence Livermore and others suggested that Jarman's explanation might be valid, no theoretical model of SBSL has explained the experimental SBSL data in sufficient detail to establish its credibility, nor has any model made predictions that can be tested.

Our Model

Our model has two basic assumptions. The first assumption is that as the bubble collapses, the gas inside is compressed and heated. This is analogous to the heat that is generated in a foot pump when it is used to fill a tire. The second assumption is that the hot gas emits light. We performed fluid dynamics simulations of the growth and collapse of a gas-filled bubble and the liquid surrounding it (Moss et al., 1997). We used the computer code LASNEX, which contains all of the physics in our model; LASNEX is also the code used for calculations of a form of thermonuclear fusion known as inertial confinement fusion, in which lasers compress a pellet to such high temperatures and densities that fusion reactions occur between atoms in the pellet.

Our calculations show that during the collapse of the bubble, a shock wave is generated that compresses and heats the contents of the bubble. More heating occurs at the center of the bubble than at its boundary because the shock wave's strength increases as it approaches the bubble's center. In the hotter regions, the atoms and/or molecule that make up the gas trapped inside the

bubble begin to break down or "ionize" into negatively charged electrons and positively charged ions. A "plasma" results—a collection of charged particles that is partially ionized. The hot gas emits light by a rapid (on the order of quadrillionths of a second) cascade of energy from the ions in the plasma, to the electrons, to the photons that make up the light pulses.

Figure 1 shows our calculated results for a collapsing argon bubble. (Our results for a collapsing air, i.e., nitrogen, bubble are qualitatively similar). Five sectors representing snapshots of the final 50 ps of the collapse are shown, during which the radius of the bubble decreases from 0.45 to 0.43 microns. Time is referenced to the instant when the shock wave reaches the center of the bubble. At –10 ps, the shock wave (red curve) is near the center of the bubble and light begins to be emitted (yellow region) just behind the shock wave. At 0 ps, the shock reaches the center of the bubble. At this point, the power (energy per unit time) that is emitted in the visible spectrum is one-half its eventual peak value. The bubble is like a miniature star: visible light from a star like the sun appears yellow, which is indicative of a temperature around 6000 K. (Hotter stars appear blue.) However, the center of the sun is much hotter, nearly 10^7 K. This temperature cannot be "seen," because the light that is emitted from the deeper regions is absorbed before it reaches the surface. This deeper absorbing region is described as being optically thick. The solid black region in the figure shows where the bubble is optically thick. Only the light emission from the halo (yellow region) and from the surface of the optically thick region can be seen. At 15 ps, the shock has reflected from the center of the bubble and is moving outward, but the gas outside the shock is still moving toward that bubble's center, compressing and heating. Consequently, the emitting halo is slightly larger, and the emitted visible optical power is at its peak value. At 25 ps, the light-emitting halo is even larger, but the bubble has cooled, so that the emitted visible optical power has decreased to one-half its peak value. At 40 ps, the bubble is too cool to emit light. The bubble temperature decreases for two reasons. First, the gas behind the outgoing shock wave expands and cools. Second, electrons carry away some of the heat that was created during the compression of the bubble. By comparing the times at which one-half peak power occurs, a 25-ps pulse width can be deduced from the figure, which is consistent with the experimentally measured value.

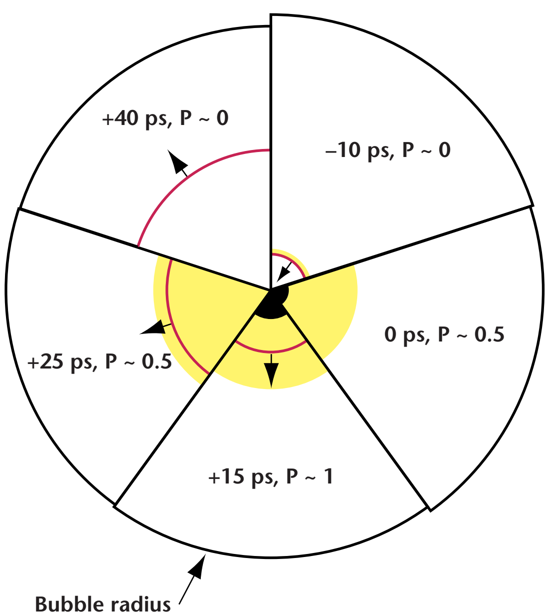


Figure 1. Our model of single-bubble sonoluminescence shows that the light-emitting phenomenon results from a shock wave inside the bubble. Here, for calculations of the final 50 ps of the collapse of an argon bubble, the shock wave location (red curve) and light-emitting regions (optically thin [yellow], and optically thick [black]) are shown. P is the relative emitted power (energy per unit time) of light in the visible part of the spectrum.

Our model agrees with many experimental results: (1) the durations of the light flashes and the spectra that they produce are

very sensitive to the maximum bubble radius; (2) the spectrum of the emitted light is described by the radiative properties of the hot gas, especially by the radiation from decelerating electrons; (3) the intensity of the emitted light from nitrogen SBSL is approximately 1/25 of that from air SBSL; and (4) the spectrum of argon SBSL is nearly identical to the measured spectrum of air SBSL, which suggests that a sonoluminescing air bubble is actually an argon bubble undergoing SL (Lohse et al., 1997) and may also explain why SBSL in noble gases (such as argon) is more intense than in diatomic gases (such as nitrogen or oxygen). Our model suggests that the mechanisms that are responsible for the ultrashort (picosecond) duration of SBSL are the electrons rapidly carrying away the energy from the bubble and the very strong temperature dependence of the emission properties of the compressed gas. Our model predicts that after the main flash, no "afterglow" will be emitted by the expanding hot bubble.

Implications for Physics Research

The physics of matter under SL conditions is not yet understood completely. Our results suggest that our basic theoretical and computational strategy is valid, and that semiquantitative predictions are possible. For example, if the collapse of the bubble can be enhanced, raising the bubble temperature even higher, then it may be possible to obtain a small amount of thermonuclear fusion from a micron-sized sonoluminescing bubble filled with heavy isotopes of hydrogen (deuterium or tritium). Although it remains to be confirmed experimentally that shock waves or plasmas are present in a bubble undergoing SL, no other model known to us has been able to explain such a broad array of experimental data.

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Predicting Complex Atmospheric Processes Using Terascale Computing Systems

William Dannevik

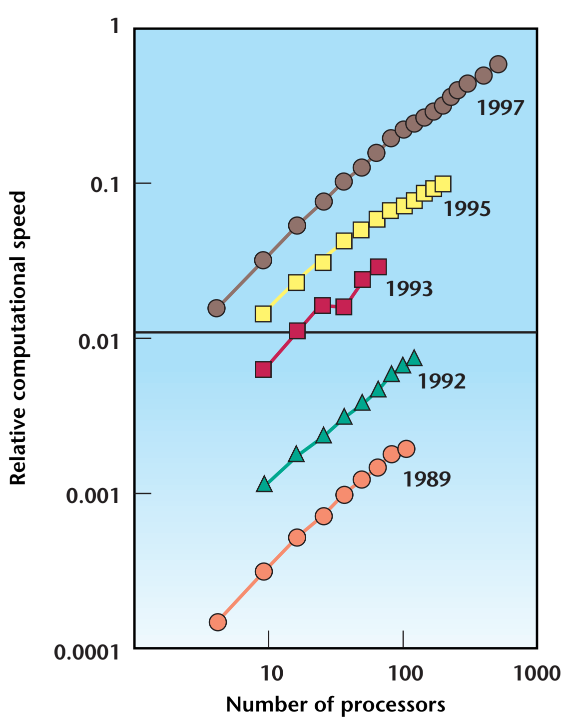
Atmospheric processes involve transient, three-dimensional interactions of many physical processes over a wide range of space and time scales. Because these processes are turbulent, multiple simulations are needed to establish the statistical significance of a single prediction. For these reasons, numerical simulations of problems such as global climate change or urban-scale dispersion of materials in complex geometries are among the most computationally demanding scientific simulation challenges.

Under the DOE Stockpile Stewardship Program (SSP), Lawrence Livermore is investing more than $100 million in masssively parallel computing systems capable of executing over one trillion arithmetic operations per second (10^{12} OPS, or one "teraops"). While the primary driver for these systems is the maintenance of the U.S. nuclear stockpile, enormous leverage exists to apply this capability to problems of national need in the earth and environmental sciences. The Atmospheric Science Division of the Earth and Environmental Sciences Directorate is developing and adapting simulation codes for execution on the SSP Accelerated Strategic Computing Initiative (ASCI) terascale computing systems.

We have been exploring the application of massively parallel computing systems to global climate simulation for several years. Over this time, the computational performance of our climate-simulation models has increased by about two orders of magnitude. With the advent of teraops computers, we expect to increase current performance by a factor of more than 100. This will enable "ensemble" simulations of climate variations on timescales of decades, using coupled models that encompass a wide range of physics processes in the atmosphere, ocean, and land surfaces. This work is already in progress with DOE and other-agency support; Livermore will play a leading role in the DOE Accelerated Climate Prediction Initiative (ACPI), to start in 1999.

We are also developing terascale simulation capability for problems in urban- and regional-scale transport and dispersion of hazardous materials by adapting U.S. Navy and other models to the ASCI platforms. The resulting state-of-art codes will support the DOE Chembio Nonproliferation and Atmospheric Release Advisory Capability Programs and the Department of Defense's Defense Advanced Research Projects Agency (DARPA) Advanced Modeling Program. To facilitate simulations that span a range of space and time scales, these models will be incorporated into a single, flexible modeling framework called the Multiscale Atmospheric Prediction System (MAPS) that will enable leading-edge atmospheric simulations.

Additional opportunities exist in earth science simulation. Subsurface reactive-transport processes are the focus of the Yucca Mountain Strategic Initiative, and other applications exist in modeling seismological and hydrological processes in heterogeneous materials.



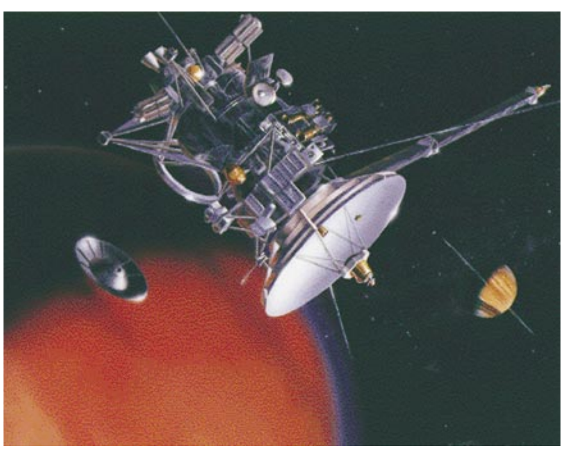
Computational speed of one of our climate-simulation models for a standard test problem, as a function of the number of processors on several generations of parallel computing systems.

The Atmospheric Release Advisory Center: NASA Mission Support

John Pace

The National Aeronautics and Space Administration's (NASA's) Cassini spacecraft, launched from the Kennedy Space Center on October 15, 1997, will enter orbit around Saturn in July 2004. Cassini will orbit Saturn for four years to study the planet and its rings, and will send a probe to the surface of Titan, Saturn's largest moon.

Cassini is carrying about 33 kilograms of plutonium-238 to supply heat and electrical power as it moves through deep space. All NASA launches involving radioactive material are provided support by the Department of Energy (DOE); DOE assigned the Livermore Atmospheric Release Advisory Center (ARAC) the task of modeling the dispersion of possible releases of radioactive material for emergency response before and during the Cassini launch. We adapted the ARAC system, which simulates the release of hazardous material into the atmosphere, predicts its movement downwind, and calculates its consequences to health, to the needs of the Cassini mission.



The Cassini spacecraft is shown in orbit around Saturn (right background) in this artist's conception. At left, the spacecraft sends a probe called the Huygens probe to the surface of Saturn's moon Titan. ARAC provided hazardous-release modeling for the launch.

Our biggest challenge was to represent the complex wind patterns in the launch area, our first (and very successful) operational use of our own execution of the Navy Operational Regional Atmospheric Prediction System (NORAPS), a weather model developed by the U.S. Naval Research Laboratory. We also used forecasts of vertical wind profiles generated by a U.S. Air Force forecaster, weather data from the many sensors arrayed around the launch area, and surface and upper air observations supplied to us by the Air Force Weather Agency.

Four ARAC scientists and three ARAC computer systems were deployed at the launch site. All model calculations were done at Livermore, but the on-site personnel assisted in interpretation of the model results and acted as interfaces to the Laboratory staff.

We made three types of plots for Cassini (dose, ground deposition, and air concentration), based on three release scenarios. We generated plots 24 hours, 3 hours, and 30 minutes before each day's launch window. At each of these times, we modeled the three release scenarios and sent one dose and one deposition plot for each scenario to NASA. These plots provided NASA officials with adequate pre-launch information.

We also generated more detailed representations that were sent to the deployed ARAC personnel to have in hand immediately if an accident were to occur. This dual approach provided access to the appropriate ARAC products for pre-launch support and any potential accident-response activities.

Fortunately, the launch went perfectly so our emergency-response capability was not needed. Because of the excellent work done by ARAC and the rapport established with NASA, we anticipate that ARAC will be asked to support any future launches involving nuclear material.

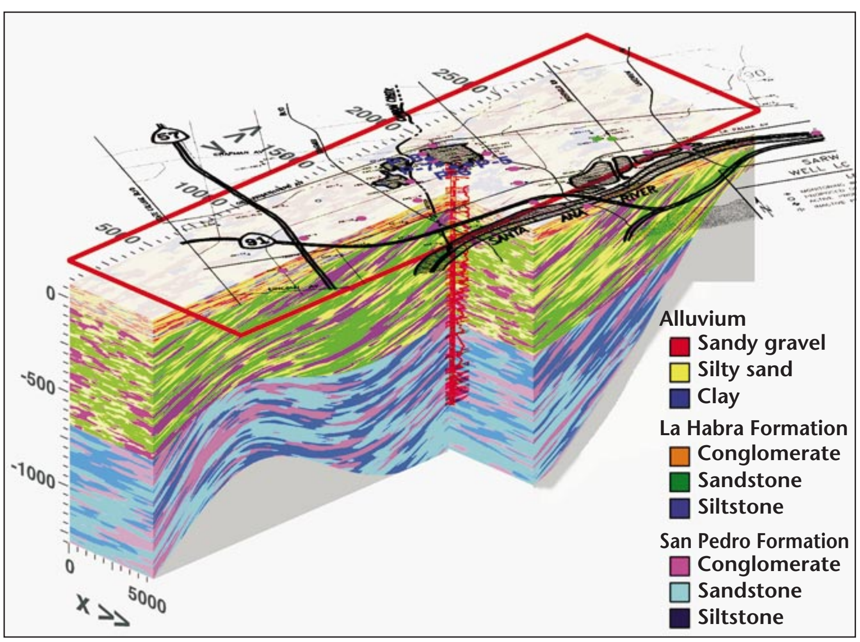
Simulation of Groundwater Migration from Artificial Recharge

Andrew Tompson

The Orange County Water District in Southern California manages one of the largest groundwater basins in the country. More than 70% of the water supply for 2 million residents is produced from groundwater resources alone, roughly 70% of which is ultimately derived from artificial recharge. Artificial recharge has historically been used to return reclaimed wastewater to the subsurface through numerous percolation basins in the district; future plans call for increasing the artificial recharge to provide a more dependable source of water. The District is strongly interested in the quality of groundwater and the impacts of historical and future recharge of reclaimed water on long-term water quality.

At Lawrence Livermore we are collaborating with the District in its water resources management by applying our unique capabilities in simulating groundwater flow and chemical migration in large, complicated, three-dimensional subsurface formations. We have developed a novel, highly detailed model of groundwater flow in the forebay area of the Orange County basin, where most of the recharge activities are concentrated. The increased spatial resolution of our model enables us to replicate finer details in the geologic structure in the formation. Simulations were used to reproduce detailed aspects of groundwater movement around thin zones of clay and silt.

The migration of recharged water was traced to estimate its residence time and travel pathways, as well as to detect what fraction of well water is derived from reclaimed water. Results were compared with estimates of groundwater age and source determined from isotopic analyses of well water. Although the model clearly showed that the age and source of the water entering the well varied with depth, the average of these ages was comparable to the apparent isotopic age that is typically determined for a mixed sample pumped from all depths. Thus, the existence of "young" water in wells must be studied further in terms of the mandated residence times (the length of time that reclaimed water must remain in the aquifer before re-use) being proposed by State authorities.



The three-dimensional geologic model developed to analyze groundwater flow for the Orange County Water District replicates fine details in structure. The model uses 45 million nodes to provide spatial resolution of 100 feet in the *X* direction, 50 feet in the *Y* direction, and 2 feet in the *Z* direction.

3-D Simulations of Earthquakes Along the Hayward Fault

Shawn Larsen

The Hayward fault runs through some of the most densely populated regions of the San Francisco Bay Area, and is estimated to have a 28% chance of generating a magnitude 6.9–7.2 earthquake within the next 30 years. It's estimated that such an earthquake could cause a disaster like that in Kobe, Japan—1000 to 10,000 fatalities, and 50 to 500 billion dollars in damage. Hence, it's critical to identify regions where high-amplitude seismic ground motions are expected so that appropriate engineering measures can be applied.

We are using high-performance computing and massively parallel processing to simulate the geographical distribution of seismic ground motion in the San Francisco Bay Area due to large earthquakes along the Hayward fault. Several earthquake scenarios have been simulated using different fault-rupture parameters including rupture direction, velocity, and amplitude, as well as slip velocity along the fault. The simulations predict that significant ground shaking will occur along the Hayward fault.

The most severe shaking is predicted for the areas around the San Pablo Bay. The San Pablo Bay overlies a deep sedimentary basin, which has the effect of magnifying the amplitude and duration of shaking. Depending on the rupture mechanism, regions at some distance from the Hayward fault could also experience significant shaking. Our calculations of ground motion are being integrated with structural models of the San Francisco Bay Bridge to assess how it will respond during a large earthquake.

These calculations are made with E3D, a sophisticated seismic-wave-propagation code developed at Lawrence Livermore. This code is being used in diverse scientific areas including earthquake research, oil exploration, nuclear test monitoring, and tectonic modeling. This explicit finite-difference code has been implemented on a number of computer platforms, from desktop workstations to massively parallel processors. Currently each earthquake simulation requires approximately 10 hours of computer time using 40 nodes of a Meiko CS-2 multiprocessor.

The simulations utilize a three-dimensional (3-D) velocity model representing the geologic structure of the San Francisco Bay Area. The model is being developed at the Seismological Laboratory of the University of California at Berkeley with support from the U.S. Geological Survey's National Earthquake Hazards Reduction Program. Our work is supported by Livermore Laboratory Directed Research and Development funds, the National Gas and Oil Technology Partnership, the Campus–Laboratory Collaborations program (CLC), the Livermore Institute for Geophysics and Planetary Physics (IGPP), and the Livermore Computations Directorate.

The Hazards Mitigation Center

Robert Murray, Paul Kasameyer, and Jean Savy

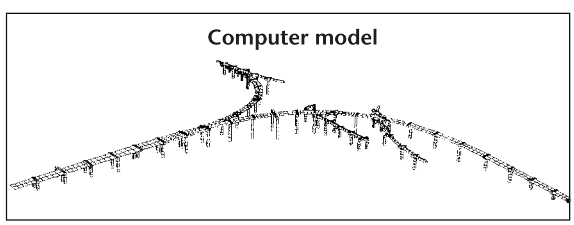
The new Hazards Mitigation Center at Lawrence Livermore integrates multidisciplinary Laboratory expertise to focus on problems of national importance that involve the study and mitigation of natural hazards (earthquakes, tornadoes, floods, high winds, lightning, and volcanoes) or anthropogenic hazards (explosions and aircraft crashes). The Laboratory has been providing expert services in this field since the 1970s. The Center establishes a point of contact and a resource center in these areas for Laboratory programs, the Department of Energy, and other agencies.

The Center integrates research, development, and application of technologies into systems for understanding and dealing with hazards—and their impacts on structures, soils, equipment, and infrastructure—from an unbiased perspective. We generate useful technical solutions to problems and, when appropriate, transfer them to industry.

The Center will be an important contributor to the nation's ability to understand, plan for, mitigate, and respond to disasters arising from natural or anthropogenic causes. We will advise government, military, and commercial disaster-planning and response organizations, as well as address energy supply and environmental security problems.

Co-directors of the Center represent the major areas of involvement: seismology, structural engineering, and hazard/risk assessment. An advisory committee has been created to help with the direction of the Center and provide support in strategic planning. Its members represent the supporting directorates at the Laboratory: Earth and Environmental Sciences, Energy, Engineering, and Computation.

Many of our current projects use three-dimensional computer simulations. For example, we are collaborating with the State of California to improve the seismic resistance of state highways, and with the University of California to study the survivability of civil structures such as bridges during large earthquakes. We are also developing prototype earthquake early-warning systems. Details of these and other projects can be found on our Web site at http://www-ep.es.llnl.gov/www-ep/ghp.html.



One of the many functions of the Hazards Mitigation Center at Lawrence Livermore is to assist state and other agencies in determining the survivability of structures such as highway interchanges in future earthquakes.

The Center for Fuels Assessment

David Layton and Douglas Rotman

Transportation fuels are a crucial component of the economic infrastructure of the United States. However, they pose a variety of health and environmental risks. Historically, it has been very difficult for regulatory agencies, as well as the automotive and oil industries, to predict and manage those risks. For example, the health and environmental impacts associated with the use of tetra ethyl lead and, more recently, methyl tertiary butyl ether, were never properly assessed before their introduction. Part of the problem is that such assessments are inherently complex and multidisciplinary and cannot be completed by multiple organizations without closely coordinated efforts.

A collaborative effort between Lawrence Livermore, Sandia National Laboratories, and the University of California can provide the coordinated expertise needed to create and implement methodologies for science-based analyses of fuels and fuel additives. To formalize this collaboration, we intend to create a Center for Fuels Assessment, whose charter will be to conduct strategic health and environmental evaluations of the nation's fuels for the 21st century. While the scientific and policy expertise found at the Laboratory and collaborating institutions provide the foundation of the Center, the execution of its charter will depend on strong links to the oil and automotive industries.

Livermore is uniquely qualified to lead this effort because we have the technical capabilities to assess the health and environmental consequences of the entire lifecycle of a given fuel or additive—its production, distribution, storage, and use. The Center's research dealing with each lifecycle element will address three fundamental topics:

(1) Quantification of contaminant releases to air, surface water, groundwater, and soil.
(2) Characterization of the transport and transformation of fuel-related substances in environmental media.
(3) Assessment of the potential health and ecological risks of those substances.

The Laboratories' expertise in these assessment topics includes both state-of-the-art computer models and experimental methods. For example, Livermore has developed sophisticated chemical kinetic models for simulating combustion products from an engine, and Sandia has a laboratory devoted to measurement of emissions produced by combustion of different fuels. An important resource is our extensive suite of models for simulating the transport of fuel-related contaminants in air, water, soil, and groundwater. Livermore's analytical capabilities for measuring contaminants in various sample matrices range from standard chromatographic techniques to the world-class Center for Accelerator Mass Spectrometry. Risk-assessment capabilities include models and experimental techniques for quantifying inhalation, ingestion, and dermal exposures to contaminants, as well as the internal doses and associated risks.

The key to establishing a successful Center will be to implement assessment methodologies that take full advantage of our capabilities and result in scientifically sound assessments of the risks posed by fuel compounds. Current efforts are directed toward defining integrated assessment methodologies and establishing collaborations with industry, government agencies and laboratories, and the University of California campuses to set the stage for interactions with potential sponsors. Our goal is to secure the funding for the Center within the next year, and begin studies that will help the nation determine the best fuels for the next century.

Investigating Mysterious Methane Hydrate

William Durham

Virtually unknown until a few decades ago, methane hydrate may turn out to be an important material in our lives. It exists in vast deposits in permafrost regions and marine sediments around the globe. If it can be recovered from such deposits, it could have a revolutionary impact on our energy budget; estimates put the carbon content of hydrate deposits at roughly twice the Earth’s total content of conventional hydrocarbon resources—coal, oil, and natural gas combined.

The deposits are also of interest because methane is a greenhouse gas, and the quantity sequestered as hydrate represents a potential environmental hazard if even a small fraction is released. Methane hydrate also poses a potential geologic hazard because it is the cement that binds some marine rock formations; its breakdown can cause undersea landslides and deadly tidal waves.

As a manufactured material, it may have applications to energy storage and transport, refrigeration, and desalinization of water. Its incidental formation in Arctic and undersea gas pipelines is a serious problem. Promoting its formation underground may provide a means for sealing “leaky” natural gas reservoirs, and avoiding sudden loss of rock strength when hydrate breaks down may open up large areas to exploration by drill bit.

Little is known about methane hydrate because it has proven difficult to recover in large amounts or to synthesize in pure form in the laboratory. Traditional methods for synthesizing gas hydrates, involving agitation of gas–water mixtures in cold, pressurized chemical reactors, invariably result in disaggregated samples contaminated with water ice. Several years ago we discovered a novel approach that involves higher pressures, no agitation, and solid rather than liquid water. The method exploits an enhanced reactivity of the grain surfaces of superheated water ice with methane and now allows us to routinely produce fully dense, pure methane hydrate samples a few tens of cubic centimeters in volume.

In late 1997 we began collaborating with the U.S. Geological Survey, supported by Livermore Laboratory Directed Research and Development funding, to investigate the physical chemistry of hydrate formation using our approach and new *in situ* methods. Our goal is to understand better why our technique works so well and how we may optimize it. Knowledge of physical properties, such as thermal and elastic properties, seismic velocities, and mechanical strength, is necessary for any attempt at surveying, mining, and handling methane hydrate and for making realistic estimates of its natural abundance. Now that we can synthesize large, pure samples, the properties can be measured using the same approaches and techniques that we currently use in rock physics.

25 millimeters

Methane hydrate—a possible future energy source—has an ice-like crystal framework that encloses gas molecules. It looks like water ice, but since it has an unusually low thermal conductivity, it does not feel as cold to the touch. Our new technique produces samples large enough to allow analysis of the material’s physical properties.

The Plutonium Immobilization Project

Henry Shaw, William Bourcier, Michael Dibley, Kevin Knauss, Sue Martin, Ron Pletcher, Keith Putirka, Frederick Ryerson, and Jesse Yow

with Roger Burns, Paul Curtis, Theresa Duewer, Bartley Ebbinghaus, Dominic Del Guidice, James Ferreira, Joseph Magana, Vicki Mason-Reed, Cynthia Palmer, Waltraud Prussin, Kevin Roberts, Vadim Romanovski, Richard van Konynenburg, and Pihong Zhao, Chemistry and Material Sciences Directorate

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Surplus fissile materials resulting from reductions in U.S. and Russian nuclear stockpiles pose a danger to national and international security because of the potential for nuclear proliferation and environmental damage. To reduce this risk, the U.S. Congress created the Department of Energy's Fissile Materials Disposition Program (FMDP) to research and implement options for rendering the surplus materials permanently unattractive for use in weapons.

One disposition option involves "immobilizing" material (plutonium) in a solid that is nuclear-criticality-safe, proliferation-resistant, and environmentally acceptable for disposal in a geologic repository. Lawrence Livermore is the lead laboratory for this immobilization option. We head a team comprising Pacific Northwest National Laboratory, Argonne National Laboratory, the Savannah River Site, the Australian National Science and Technology Organization, and others in a program of research, development, and testing that will result in operation of a plutonium-immobilization plant by 2005 or 2006. The Nonproliferation, Arms Control, and International Security Directorate oversees these activities at Livermore, and the Earth and Environmental Sciences Directorate provides technical management and scientific expertise in wasteform development, testing, and modeling.

In 1997, following 18 months of research, we compared the relative merits of two candidates for plutonium immobilization: a lanthanide-rich borosilicate glass and a titanate-based ceramic. The candidates were compared using criteria previously used by the FMDP: (1) resistance to theft, diversion, and recovery of plutonium by a terrorist organization or rogue nation; (2) resistance to recovery and reuse by the host nation; (3) technical viability; (4) environmental, safety, and health factors; (5) cost effectiveness; and (6) timeliness.

Though both materials were found to be acceptable, the ceramic technology was recommended because of several advantages over glass:

- Greater robustness to the threat of theft, diversion, and reuse.
- Higher durability in a repository environment.
- A significantly lower radiation source term, reducing the potential for worker exposure during fabrication.
- Potential cost savings.
- A more flexible technology, and possibly greater ability to accommodate modifications to programmatic and technical requirements.

The ceramic is based on a pyrochlore-structured phase, with subsidiary hafnium-zirconolite and minor amounts of brannerite and hafnium-bearing rutile. Our present work is aimed at demonstrating the tolerance of this formulation to impurities. The plutonium-bearing minerals are being tested to determine the mechanisms of reaction with groundwater, and to determine which secondary phases may form from degradation of the ceramic. The distribution of fissile nuclides and neutron absorbers among the secondary phases, and their aqueous solubilities, are being characterized. Models for the reaction rate as a function of temperature and solution composition are being developed. Future work will use plutonium-238-doped ceramic and ion-bombardment techniques to study the effects of radiation damage on the performance of the ceramic.

Bioscience Nuclear Microscopy

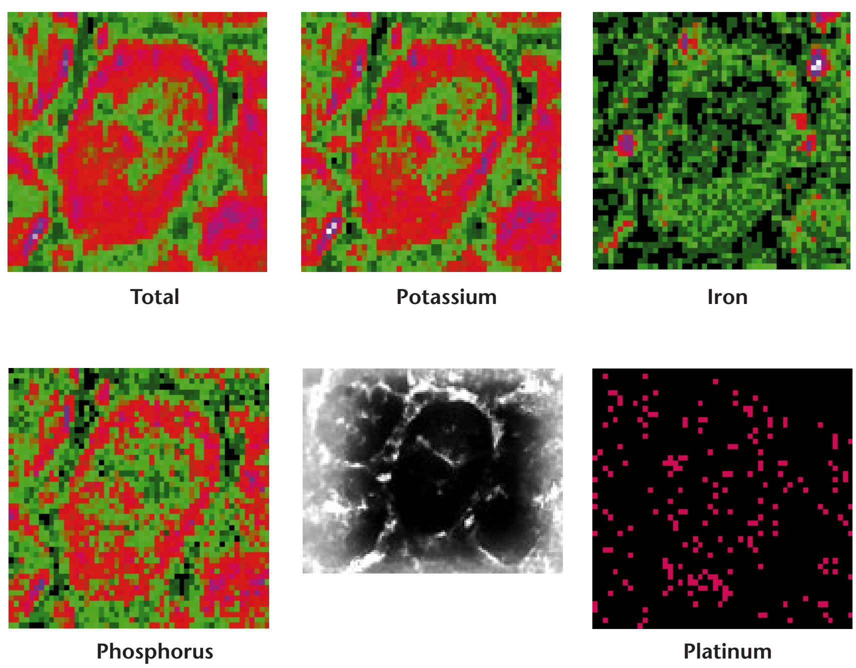
Graham Bench, Patrick Grant, and Stephanie Jeske

The roles that metals play in health are an increasing concern. Unfortunately, understanding of these roles is hindered because the analysis techniques in current use cannot accurately quantify the spatial resolution of metals in biological matrices. Bioscience needs to adopt a technique that can measure metal distributions at the sub-cellular level.

Lawrence Livermore is well positioned to undertake development of such a technique—bioscience nuclear microscopy. This work enhances the Earth and Environmental Sciences directorate's core competencies in two areas: (1) pathway, dosimetry, and risk analysis of radioactive and toxic substances, and (2) ion-beam and isotopic sciences. Furthermore, we can draw on our collaboration with researchers in the Biological and Biotechnology Research program who have recognized expertise in biological fields. This collaboration on projects requiring quantitative elemental microanalysis helps develop proper protocols for sample analysis and addresses the impact of the technique on proposed study areas.

Nuclear microscopy can measure elemental profiles quantitatively and accurately at the micron scale at sensitivities approaching the part-per-million level (sensitivities approaching 10 attomoles in individual cells). A combination of proton-induced x-ray emission and scanning transmission ion microscopy are used to generate element-concentration maps and histological information. Applications include environmental tracing, toxicology, carcinogenesis, and structural biology.

In the past year we have refined sample-preparation methods that enable elemental microanalysis to accurately represent tissue *in vivo* (this includes methods for growing and freeze-drying cell cultures on thin foils and establishing procedures for tissue sections). We have determined minimum detection limits and sensitivities for a range of metal toxins, carcinogens, and cancer-treating drugs in a variety of tissues. We have also addressed current concerns in biology through our collaborative projects. These projects include: study of factors controlling central-nervous-system transport and toxicity of inhaled inorganics and radionuclides; quantification of specific microenvironments within cultured phagocytic cells and assessment of changes that occur during infection with *Salmonella typhimurium*; study of the effect of sperm protein and metal defects on male fertility; renal uptake of cancer-treating platinum-containing drugs; and design of a rapid and accurate assay for hazardous metal uptake by skin.



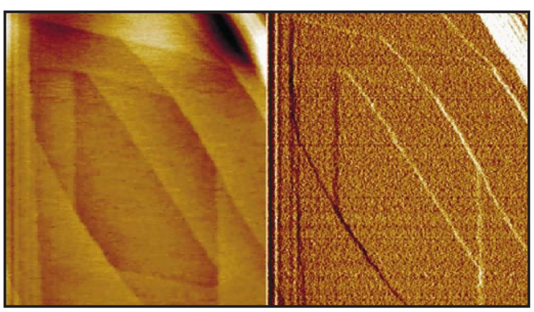
Bioscience nuclear microscopy allows accurate spatial resolution of metals in tissue. Here, a rat kidney tubule is imaged for study of the uptake of the cancer-treating drug cis-platinum. (The therapeutic effect of the drug is limited in part by its nephrotoxicity.) The color images display x-ray distributions; colors indicate element concentrations. The black and white image is an optical micrograph of the same area after analysis; the darkened region shows areas irradiated with the microbeam.

Atomic Force Microscope for Imaging under Hydrothermal Conditions

Kevin Knauss, Carl Boro, Steven Higgins, and Carrick Eggleston

Scanning probe microscopy, comprising scanning tunneling microscopy (STM), atomic force microscopy (AFM), and related techniques, has become an indispensable tool for imaging solid surfaces at resolutions ranging from the atomic scale (for periodic and defect structures) to the microtopographic scale (for roughness, step-terrace patterns, magnetic patterns, microorganisms and biomolecules, etc.). AFM is also important for crystal-growth studies because it allows not only *ex situ* characterization of the spacing and shape of atomic-scale steps and terraces, but also *in situ* real-time imaging of step motion and surface kinematics during crystal dissolution or growth in aqueous or other solutions.

A limitation of AFM has been the relatively narrow range of temperatures accessible for *in situ* imaging in aqueous solution. The range of crystal dissolution or growth rates accessible to *in situ* AFM imaging of step motion is about 10^{-6} to 10^{-10} moles meter^{-2} second^{-1}. Rates for most oxides and silicates (of interest in applications such as chemical weathering of rocks and buildings, radioactive waste storage, industrial pipe scaling, and enhanced oil-recovery techniques such as steam-flooding) are slower than this range at room temperature. In order to apply AFM to the aqueous dissolution and growth of these materials, higher temperatures are needed.



In situ **AFM images cropped from a movie of barite dissolving at 150°C under flowing conditions in a pH 2 solution. These movies of etch-pit sub-nanometer monolayer motion are used to measure dissolution kinetics and the energy of the dissolution or growth process as a function of crystal orientation.**

We have designed and constructed a contact atomic force microscope that can be used to image solid surfaces in flowing aqueous solution up to 150°C and 10 atmospheres pressure. The main features of this unique AFM are: (1) an inert-gas-pressurized microscope base containing a stepper motor for coarse advance and a piezoelectric tube scanner; (2) a chemically inert membrane separating these parts from the fluid cell; (3) a titanium fluid cell with fluid inlet–outlet ports, a thermocouple port, and a sapphire optical window; (4) a resistively heated ceramic booster heater for the fluid cell to maintain the temperature of solutions sourced from a hydrothermal bomb; and (5) mass flow and pressure control. The design overcomes current limitations on the temperature and pressure range accessible to AFM imaging in aqueous solutions. We have successfully imaged calcite, barite and hematite at high temperature and pressure, demonstrating unit-cell-scale (<1 nanometer) vertical resolution of the AFM under hydrothermal conditions.

To our knowledge, this is the first report of an AFM design with these novel capabilities.

The Geographic Information Sciences Center

Charles Hall

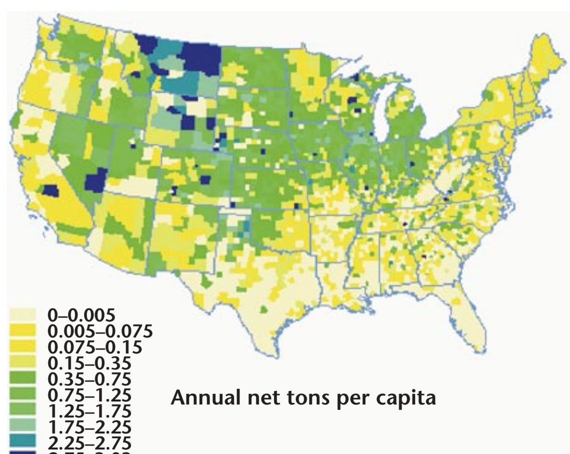
Many research problems involve environmental, physical, or temporal parameters tied to a specific geographic location. The Geographic Information Sciences (GIS) Center is an important capability for analyzing these complex planning, resource management, and research problems. Our mission is to offer a cost-effective combination of personnel, hardware, and software for acquiring, managing, analyzing, and displaying spatially referenced data. Specific applications include environmental and human health risk; geophysical, atmospheric, and hydrologic modeling; environmental restoration; facilities management; energy research; national and international security; and emergency response issues.

A geographic information system is essential for analyzing the relationships among parameters in these kinds of problems to enhance understanding of the phenomena being observed or modeled. The GIS Center provides a very powerful, complex system comprising a significant investment in hardware; software; network and storage facilities; and high-quality data control, formatting, and library organization and maintenance. The Earth and Environmental Sciences Directorate is making this substantial resource available to all interested researchers. Our goal is to work side by side with researchers, providing baseline data and expertise in geospatial analysis, integrating project-specific data, and refining analyses and output graphics.

We use a relational database of environmental, demographic, infrastructure, and other spatially referenced data to which structured queries and statistical analyses can be applied. The relationships among the many layers of information are analyzed and the results are usually displayed in map form. We can prepare map and plot output for publication, produce large-format posters, and support presentations with projected computer-generated maps and graphic output.

Projects that we have completed include a map displaying sample sites and isopleths of cesium deposition in the western United States resulting from activities at the U.S. Nevada Test Site in the 1950s and 1960s. We are also supporting a researcher in an investigation of the relationship between radon and lung cancer. We have compiled a large set of physical and socioeconomic data and are calculating the population-weighted average elevation for every county in the United States. We are developing a GIS-supported algorithm for estimating the location of a toxic spill in which the onset of adverse health symptoms is delayed. We are pursuing initiatives in support of other projects involving locating and managing toxic substances.

The Center is creating and cataloging an extensive geospatial data library accumulated by researchers; with their approval, it will be made available on the Internet.



Resources in the GIS Center's database are available for research on location-specific problems; this map of bituminous coal use in the United States in 1918 was created from historical data for use in investigating the relationship between radon and lung cancer rates.

Resources: An Overview of the Earth and Environmental Sciences Directorate

The Earth and Environmental Sciences Directorate operates programs and pursues basic and applied research across the Laboratory's three major program areas:

- Environmental change and remediation.
- National and civil security.
- Health risks and natural and anthropogenic hazards.

To achieve these goals, the management team for Earth and Environmental Sciences strives to:

- Staff with talented, motivated scientists, engineers, and administrative personnel.
- Execute good business practices and continually review financial systems.
- Maintain and enhance high-quality facilities with an emphasis on maintaining an excellent safety record.

Workforce

Our directorate currently employs 262 people (Figure 1). Of this total population, about 73% are scientists and engineers with a wide range of specialties, which are listed in Table 1. In addition, this workforce is complemented by personnel from other Livermore organizations, such as Engineering and Computation, who are assigned to support the directorate's mission. The total number of people working with and

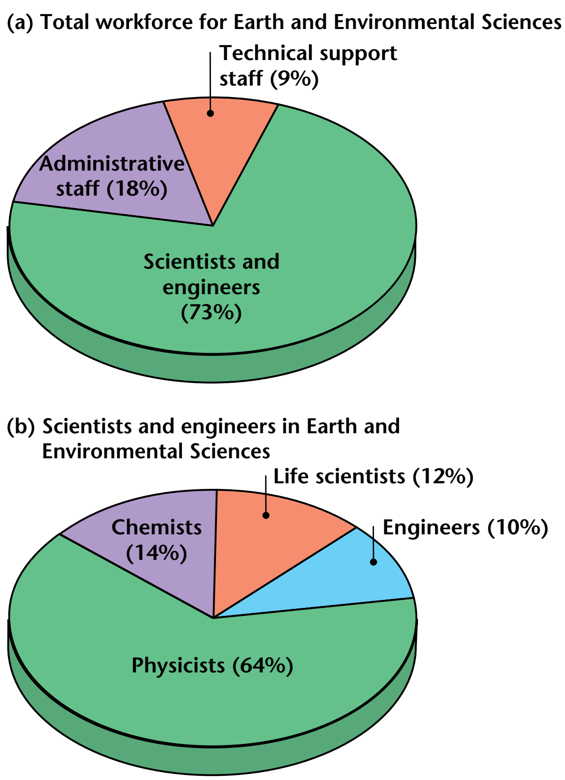


Figure 1. Workforce breakdown for Earth and Environmental Sciences. (a) Total workforce is 262 employees, of which (b) 190 are scientists and engineers.

Table 1. Discipline specialties within the Earth and Environmental Sciences Directorate.

Discipline	Research specialties
Physics	Accelerator applications, astrophysics, atomic, computational, solid state, theoretical, materials, biophysics, and geophysics. Staff also include specialists in meteorology, atmospheric science, seismology, hydrology, geology, physical properties of rocks, climatology, and oceanography.
Chemistry	Isotope, theoretical, nuclear, organic, biochemistry, and geochemistry. Staff also include specialists in marine, agricultural, physical, ecology, and soil chemistry.
Life sciences	Environmental science, environmental health, forestry, biology, plant science, microbiology, radiobiology, toxicology, water resources, wildlife, marine and fishery biology, and zoology. Staff also include a medical doctor, an environmental lawyer, a geographer, a social scientist, and an economist and anthropologist.
Engineering	Mechanical, electrical, civil, geotechnical, environmental, marine, nuclear, geological, and chemical engineers. Staff also include specialists in mining, applied science, aeronautical, industrial, and cybernetics systems.

within Earth and Environmental Sciences makes this one of the largest environmental research organizations in the nation.

Funding

The directorate's workforce supports a diverse set of programs and projects (see Figure 2). In 1997, the total funding from all sources was $66.1 million, including a $4.2 million allocation from the Laboratory Directed Research Development Program. Several programs at the U.S. Department of Energy sponsor our projects directly ($27.8 million in 1997). These programs include Environmental Restoration and Waste Management, Energy Research, Defense Programs, Environmental Health and Safety, and others (International Affairs and Nuclear Reactors). We also received $8.4 million in support of Work for Others, including funding from Department of Energy field offices and integrated contractors; from other federal agencies, such as the U.S. Navy, Air Force, and Department of Defense and the National Aeronautics and Space Administration (NASA); and from private industry and universities, such as California State University. In addition to direct funding to this directorate, in 1997, we received $25.7 million through other Livermore directorates for program management and expertise provided by our personnel. These included the Comprehensive Test Ban Treaty Program and the proposed repository at Yucca Mountain, Nevada.

The directorate is a composite of environmental sciences, geophysics, atmospheric physics, and other scientific disciplines. Listing the funding sources does not describe the diverse nature of our research. Thus, in Figure 3, we show the breakdown of funding by project or program.

In recent years, Livermore has continued to streamline its management and financial practices to reduce infrastructure costs and

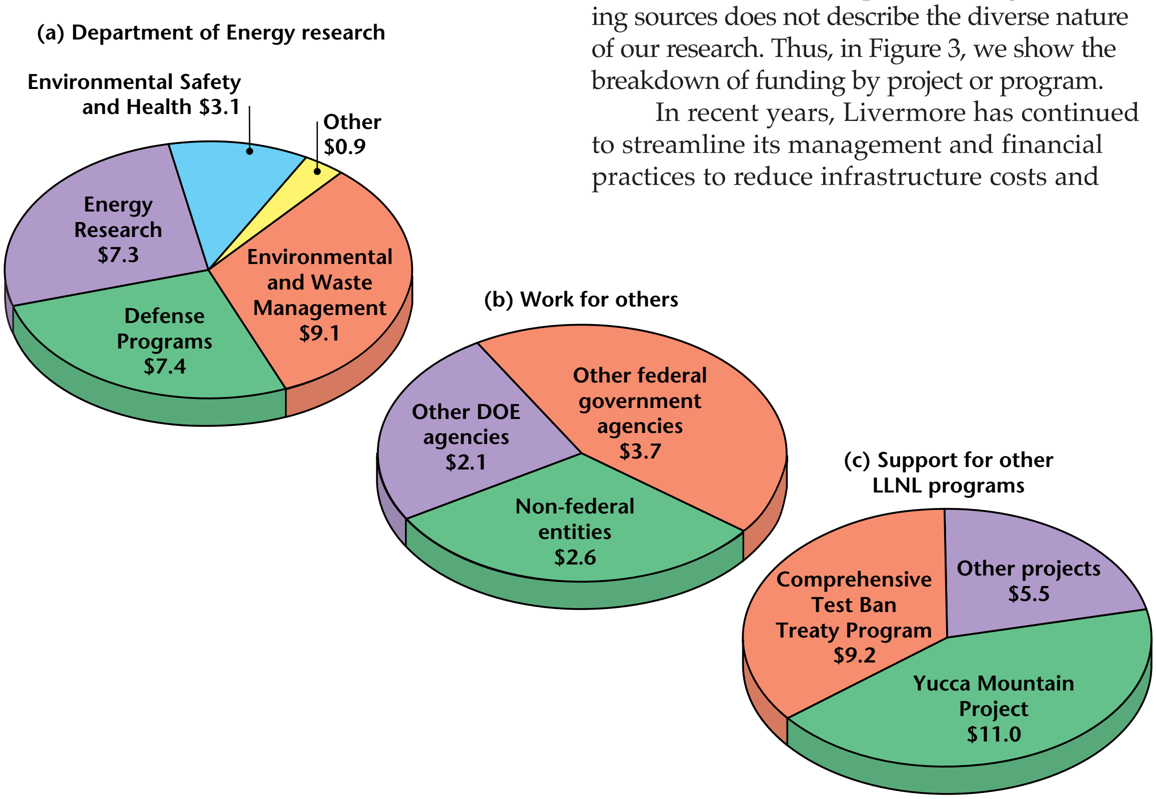


Figure 2. Breakdown of funding for Earth and Environmental Sciences in 1997 (in millions of dollars). (a) Funding received directly from the Department of Energy totaled $27.8 million. (b) Funding received in work for others totaled about $8.4 million. (c) Funding received to provide program management and scientific expertise for other Lawrence Livermore programs totaled $25.7 million.

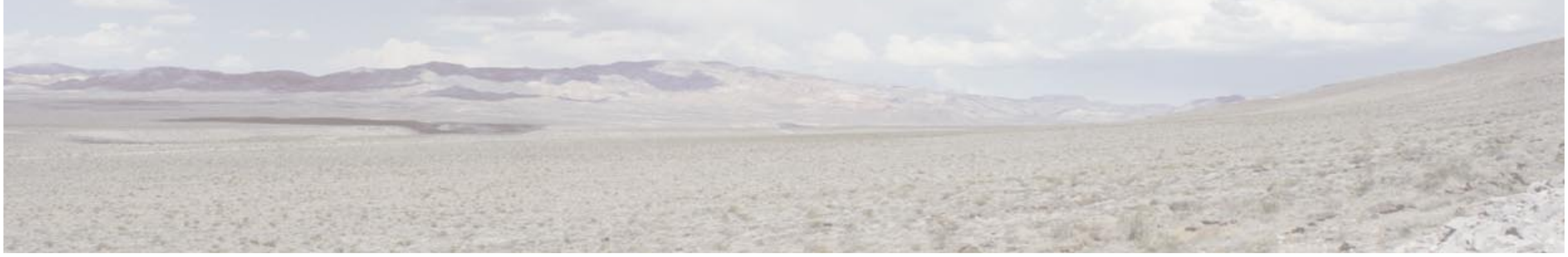
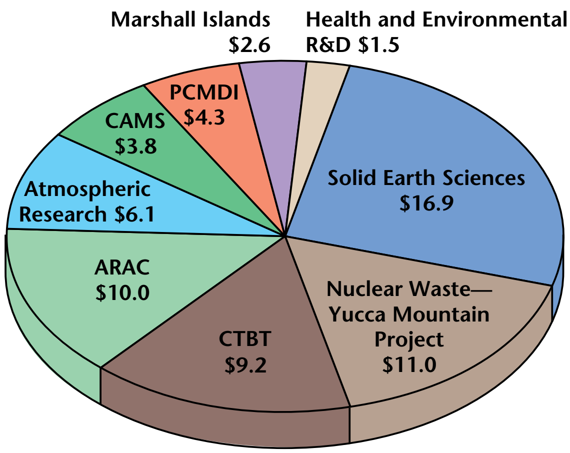


Figure 3. Breakdown of 1997 funding by program or project. Amounts are in millions of dollars. PCMDI = Program for Climate Model Diagnosis and Intercomparison, CAMS = Center for Accelerator Mass Spectrometry, ARAC = Atmospheric Release Advisory Center, CTBT = Comprehensive Test Ban Treaty Program.



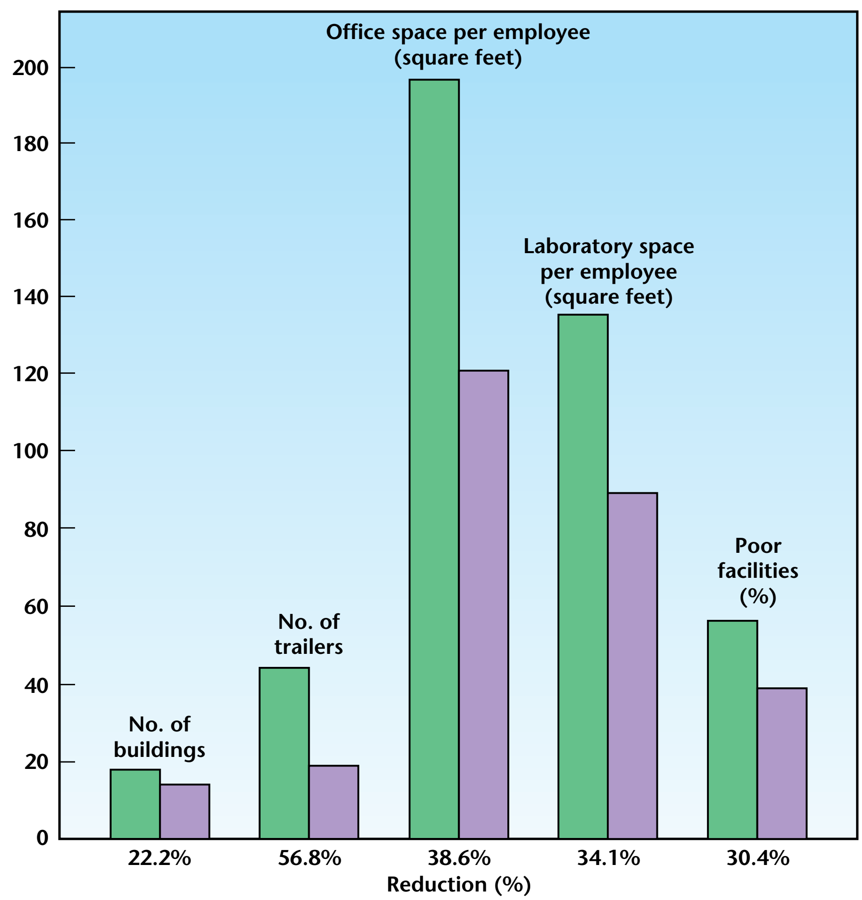


Figure 4. Consolidation of facilities in Earth and Environmental Sciences between 1995 (green) and 1997 (purple). We are now at acceptable norms for the directorate to function smoothly and efficiently.

make procedures less cumbersome. The Laboratory and the Directorate continue to take every opportunity to monitor and control cost expenditures to stay efficient and cost-effective. The commitment to reduce infrastructure costs has led to decreases in G&A spending, procurement charges, and overhead costs and rates.

Facilities

We continue to make significant progress in our space-consolidation process, begun when the directorate was formed in 1994. The challenge we continue to face is how to balance the available funds for space with plans for the future operations of the directorate. Our goal is to consolidate these facilities to improve the directorate's operations and its programmatic capabilities while minimizing one-time moving expenses and recurring overhead costs.

Our aggressive facilities management has achieved an enormous increase in efficiency by reducing our total number of facilities from 62 in 1994 to 33 in 1997, and total space from 300,000 to 200,000 square feet. We kept 1997 overhead space costs for the directorate at the 1996 level—$1.2 million (down from $1.8 million in 1994). We also improved our use of the available space and thus the efficiency of our operations, and by vacating obsolete buildings we reduced the directorate's maintenance burden. Figure 4 shows our 1995–1997 accomplishments in reconfiguring and optimizing the directorate's facilities. In both office space and net space per person housed, we are well below the Laboratory averages. The directorate's six primary facilities are described in Table 2.

In the future, we plan to complete the consolidation process and release any remaining underused or low-quality space. An important focus is the replacement and renovation of the trailer complex that currently houses nearly 200 directorate and associated personnel. We also plan to improve the capabilities of key facilities to

Table 2. Major facilities in the Earth and Environmental Sciences Directorate.

National Atmospheric Release Advisory Center, Building 170
- 44,000-square-foot facility
- Commissioned on February 26, 1996
- Award for architecture
- Fitted throughout with fiber-optic communication links
- 120 offices, a library, and a conference and training center

Center for Accelerator Mass Spectrometry, Building 190
- 9,000-square-foot facility
- Multi-user Tandem Laboratory
- Houses two accelerators
  - One 10-megavolt model FN Tandem Van de Graaff
  - One newly installed 1.8-megavolt Tandem for particulate research
- Broad variety of applied research using ion-beam analysis and accelerator mass spectrometry

Health and Ecological Assessment Laboratories, Building 281
- 19,000-square-foot facility
- An older existing facility that was extensively renovated during 1996
- Used to consolidate closely related programs and experiments from six geographically separate facilities
- Includes both wet and dry chemistry, laser, and high-pressure laboratories and support space

Molten Salt Oxidation Demonstration Project, Building 292
- 3,500-square-foot facility
- Used to study performance of an integrated molten salt oxidation (MSO) system including primary unit, offgas, and salt recycle subsystems
- Construction completed and experimental work began in September 1997

Geoscience Technologies Laboratories, Building 243
- 18,000-square-foot facility
- Includes wet and dry chemistry, laser, and high-pressure laboratories, as well as a machine shop and support areas
- Used to conduct research in support of basic energy sciences, fossil energy projects, the Yucca Mountain project, the Accelerated Site Cleanup project, the Environmental Technology program, and other Laboratory-directed research and development

Environmental Microbial Biotechnology Facility, Building 446
- 1600-square-foot facility
- Includes a 1500-liter bioreactor and dedicated ancillary equipment
- Ability to grow, harvest, and radioactively label specific bacteria for bacterial cell or cellular DNA labeling and containment studies
- Used to conduct research in support of the Yucca Mountain Project, bioremediation, and microbial transport.

enhance programmatic success. As a result, we hope to continue to be one of Livermore's lead organizations in cost-effective research and programmatic operations.

Organization

Figure 5 shows the organization of Earth and Environmental Sciences. The major components are (1) the four divisions, which contain the scientific and support staff and have principal responsibility for the execution and maintenance of disciplinary science; (2) the project organizations, which execute focused missions for this directorate and others at Lawrence Livermore; and (3) the infrastructure activities, which support our research and programmatic efforts. Each of these three components has a vital role to play in creating and nurturing an organization that is scientifically excellent, capable of accomplishment that impacts national issues, and is safety conscious, cost-effective, and agile in the current climate of national science and technology. A point particularly worth noting is the correlation between the Special Programs in Figure 5 and the breakdown of funding shown in Figure 3. The project

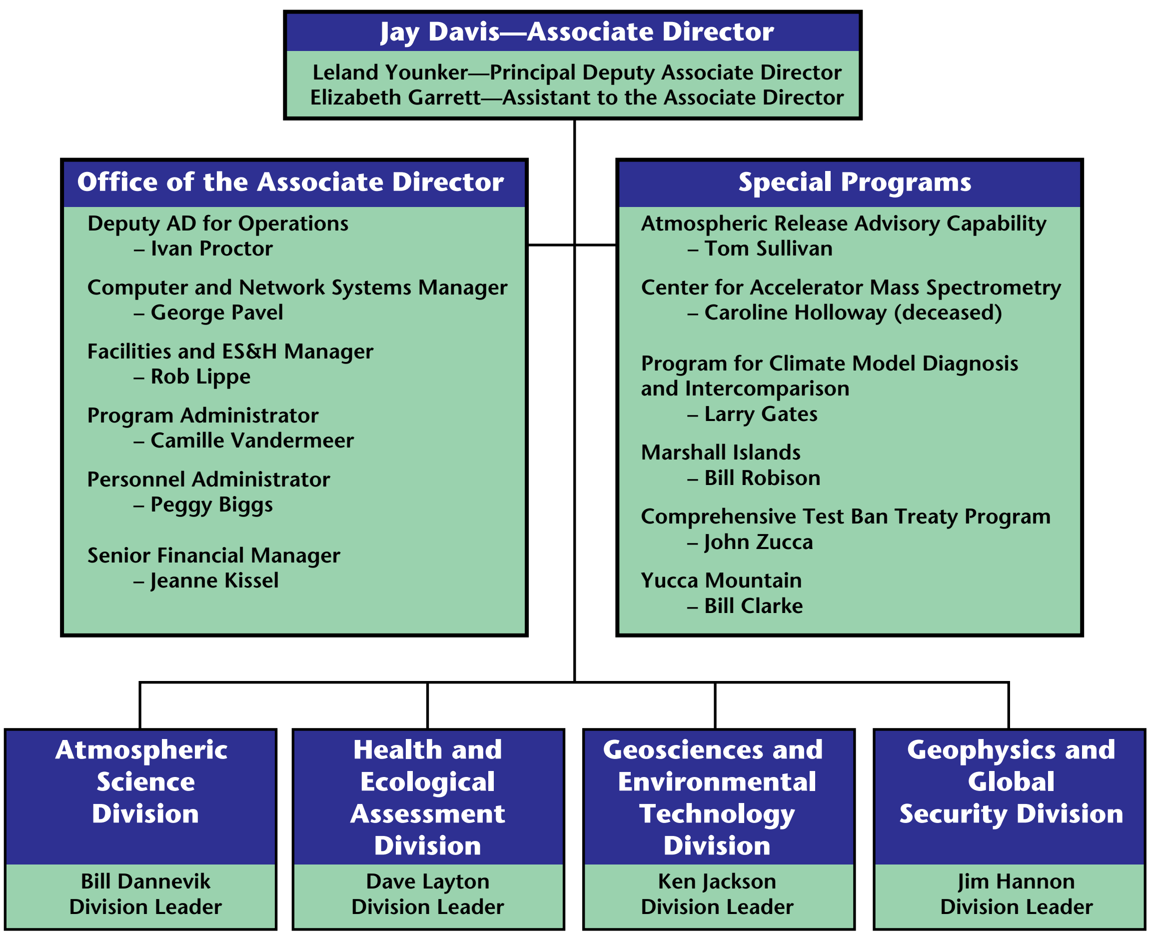


Figure 5. Organization of the Earth and Environmental Sciences Directorate.

organizations control a major fraction of the directorate's resources. The mission and capabilities of each division are described on the following pages.

Atmospheric Science Division

The mission of the Atmospheric Science Division is to expand scientific understanding of how Earth's atmosphere, oceans, and biosphere respond to the anthropogenic and natural disturbances that contribute to environmental risk. To meet the demands of contemporary environmental problems, the division maintains expertise in:

- Atmospheric dynamics, chemistry, and physics.
- Ocean dynamics, transport, and biogeochemistry.
- Mesoscale atmospheric prediction, transport, and dispersion.
- Hydrology and terrestrial ecology.
- High-performance computing and computational physics.

This expertise is combined with the best available environmental simulation models, observational and real-time datasets, and computing resources to examine a range of problems. For example, our studies include the transport and dispersion of hazardous materials released into the atmosphere, global- and regional-scale impacts of changes in atmospheric chemical composition, variations in the Earth's climate and carbon cycle, and regional-scale variations in hydrological processes. The division also provides the technical staff for two major programs: the Atmospheric Release Advisory Center, and the Program for Climate Model Diagnosis and Intercomparison.

For more information on Atmospheric Science, contact the division leader,
Bill Dannevik, at (925) 422-3132 (dannevik1@llnl.gov).

Health and Ecological Assessment Division

The basic mission of the Health and Ecological Assessment Division is to conduct research to assess and manage the risks of chemicals in the environment. The Division's core expertise in the health, ecological, and measurement sciences provides a strong basis for multidisciplinary studies of toxic and radioactive substances released to the environment. An important asset of this division is a unique set of research facilities, which include:

- Laboratories for processing soil and vegetation samples for subsequent analysis.
- Alpha and gamma spectrometry for determining low levels of radionuclides in environmental media.
- Gas chromatography and high-performance liquid chromatography for measuring various organic compounds in different media.
- Atomic absorption spectrometry for analyzing metals.
- Accelerator mass spectrometry and proton-induced x-ray fluorescence for quantifying selected nuclides (such as ^{14}C, ^{129}I, ^{36}Cl, ^{59}Ni) and various elements.

Our measurement technologies support a broad range of field and laboratory studies within the HEA Division and the E&ES Directorate. We have also developed both experimental methods and computer models to assess the nature and magnitude of human exposures to chemical contaminants via inhalation, dermal contact, and ingestion. An important asset is our considerable experience in constructing dose-response functions for estimating the risk that such contaminants pose to humans. We also perform detailed studies involving the environmental chemistry and toxicology of various kinds of organic and inorganic substances, and we develop methods for managing the risks they pose to humans and ecosystems. We are equipped to characterize pollutant-transport processes, such as the resuspension of contaminants deposited

on soil. Finally, we conduct large-scale field programs, develop remote-sensing technology, establish environmental databases, and create geographic information systems.

For more information on Health and Ecological Assessment, contact the division leader, Dave Layton, at (925) 422-0918 (layton1@llnl.gov).

Geosciences and Environmental Technology Division

The Geosciences and Environmental Technology Division conducts basic and applied research to solve problems involving the geochemistry, geophysics, and flow and transport properties of the Earth's near-surface, and to develop or improve the nation's waste-disposal and waste-processing technologies. The Division's research is focused in five basic areas:

- Subsurface characterization, especially the development of new geophysical and electromagnetic methods for characterizing the physical and chemical properties of the shallow subsurface, and for identifying and mapping contaminant plumes.
- Subsurface remediation, with emphasis on developing novel techniques for the accelerated *in situ* cleanup of subsurface contaminants as well as integrated assessment and cleanup strategies.
- Nuclear waste disposal, including characterization and modeling of the thermally perturbed geochemistry, hydrology, and transport mechanisms of high-level nuclear waste repositories. We also design and test different disposal strategies, and model how various nuclear waste forms will react once emplaced into a repository.
- Waste-processing technologies, including the development and testing of systems that provide alternatives to incineration for treating and stabilizing mixed hazardous and nuclear wastes.
- Basic geosciences research, such as studying the dissolution kinetics of minerals and glasses, the thermodynamic and transport properties of aqueous geochemical systems, developing geologic information systems, and applying cosmogenic isotopes as tracers and age-dating tools.

For more information on Geosciences and Environmental Technology, contact the division leader, Ken Jackson, at (925) 422-6053 (jackson8@llnl.gov).

Geophysics and Global Security Division

The mission of the Geophysics and Global Security Division is to conduct basic and applied research that characterizes the physical and chemical properties and processes of the solid Earth and to use the results of the research to address challenges to national security, civic infrastructure, and industry. The challenges include natural and anthropogenic hazards; test ban treaty violations; production of geothermal, oil, and gas energy; and containment of radioactive materials. The Division's primary areas of research are:

- Seismology, including empirical and computational studies of source and propagation effects on local, regional, and teleseismic ground motion, and signal processing, discrimination, and regional characterization in support of verification of a Comprehensive Test Ban.
- Computational physics, including shock physics, computer modeling, information sciences, weapons physics, sonoluminescence, and theoretical and applied physics.
- Experimental physics, including synthesis of materials; rock mechanics; flow in porous materials; physical and chemical properties of earth materials, cementitious materials, and metals at high pressures and temperatures; and experimental design.

- Geophysical site characterization, including theoretical and applied geophysics, geomechanics, engineering, containment science, field operations, on-site-inspection technologies, and instrumentation.

Division personnel provide the direction for a wide variety of Laboratory programs including Comprehensive Test Ban verification, Containment, Geothermal, Basic Energy Science, and Remote Sensor Test Range Programs, the Hazard Mitigation Center, and a significant element of the Yucca Mountain Program.

For more information about the Geophysics and Global Security Division, contact the division leader, Jim Hannon, at (925) 422-6452 (hannon2@llnl.gov).

Outreach and Collaboration

Research and development in the Earth and Environmental Sciences Directorate is funded by a wide range of federal agencies, and the Directorate interacts with academic, industrial, and national laboratory organizations working in the earth and environmental sciences. As in the past, no one agency or organization dominates this area, and the expertise required to be a significant contributor is multifaceted. Over this past year, Earth and Environmental Sciences has increased its collaborations with other LLNL Directorates and the external community.

Our exposure to a large outside community allows us to assess our strengths and provides challenges for improvement. It provides insights into the strengths of other groups at the earliest stages of their development, and provides a means to demonstrate our strengths through interactions. This exposure complements that obtained from our more formal activities such as publications and workforce proceedings.

Major components of outreach in 1997 include the following:

- Approximately 500 ongoing and new collaborations with external researchers occurred (increased from 170 in 1996).
- More than 65 faculty members and students and 78 other scientists visited for stays of more than a week.
- 60 students participated in eight on-site work-study programs.
- About 40 conferences or workshops were organized or hosted.
- 168 groups toured our facilities, predominantly ARAC and CAMS.
- More than 140 Directorate employees participated on major national and international committees and review panels, or served as visiting lecturers, or journal associate editors and reviewers.
- 38 summer students were hired during the summer of 1997, including 19 women and many minorities, from a variety of academic institutions and programs.
- Two campus–Laboratory Cooperation projects involved participation with several University of California campuses.
- 12 E&ES projects involving UC faculty and students were sponsored through the Livermore Institute of Geophysics and Planetary Physics.
- More than 100 employees participated in community activities such as special instruction, computer programs, classroom training, mentoring students, workshops and special conferences, community service campaigns, etc.

These outreach and collaboration efforts are important contributions to the Directorate's development and its ability to contribute to and profit from the larger technical community and society as a whole. Although we have not established specific performance measures for employees participating in these areas, such participation is a factor in our evaluation of the employees' professional development and their value to the Laboratory. The communication provided by such interactions is essential if we are to improve our strengths, correct our weaknesses, make our efforts relevant to society, and receive recognition for work well done.

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Awards and Patents

Awards

William Durham (and two co-researchers from the U.S. Geological Survey) won the Richard A. Glenn Award from the Division of Fuel Chemistry of the American Chemical Society.

Steven Hunter (Electronics Engineering) and Carl Boro won an R&D 100 Award for their oil-field tiltmeter.

A co-researcher with William Moss on the Sonoluminescence Project, Tom Matula of the University of Washington, Applied Physics Laboratory, was awarded the DOE Defense Programs Young Scientist and Engineers Award. He was also nominated by Defense Programs for the Presidential Early Career Award for Scientists and Engineers, and received that award.

W. Lawrence Gates received the DOE Biological and Environmental Research Program Recognition Award, in recognition of his initiation of the concept of climate-model intercomparison studies to systematically ascertain and correct model bias and errors, at a symposium co-sponsored by DOE and the National Research Council, "Serving Science and Society: The Legacy and the Promise of the Agency's Biological and Environmental Research."

Roger Aines, Marina Chiarappa, Allen Elsholz, Bryant Hudson, Gene Kumamoto, Roald Leif, and Robin Newmark were presented with the Livermore Director's Performance Award honoring their leadership in teaming with three directorates and the Southern California Edison Company to field-test the hydrous pyrolysis/oxidation concept on a full scale.

Patents

Patent issued to	Patent title, number, and date of issue
Roger Aines* Robin Newmark*	**Active Cooling-Based Surface Confinement System For Thermal Soil Treatment** U.S. Patent No. 5,681,130 (IL-9479 [RL-12,666]) October 28, 1997
Joseph Lucas Tore Straume* Kenneth Bogen*	**Detection and Isolation of Nucleic Acid Sequences Using Competitive Hybridization Probes** U.S. Patent No. 5,616,465 April 1, 1997
Ananda Wijesinghe* et al.	**Nontoxic Chemical Process for In-situ Permeability Enhancement and Accelerated Decontamination of Fine-Grain Subsurface Sediments** U.S. Patent Number 5593248 January 14, 1997

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